



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2022 – 12:23 PM EST

PDB ID : 2H35
Title : Solution structure of Human normal adult hemoglobin
Authors : Fan, J.S.; Yang, D.
Deposited on : 2006-05-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

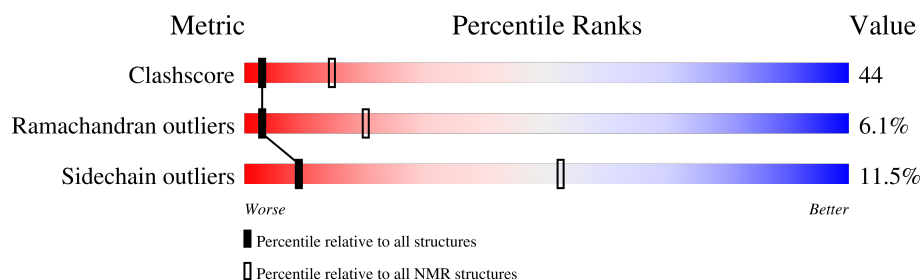
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	141	<div> <div>34%</div> <div>54%</div> <div>8%</div> <div>.</div> </div>
1	C	141	<div> <div>33%</div> <div>54%</div> <div>9%</div> <div>.</div> </div>
2	B	146	<div> <div>58%</div> <div>39%</div> <div>..</div> </div>
2	D	146	<div> <div>57%</div> <div>40%</div> <div>..</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:41, A:45-A:138, B:2-B:146, C:1-C:41, C:45- C:138, D:2-D:146 (560)	0.57	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 10, 11, 12, 18
2	4, 8, 16, 17
3	9, 13, 14
4	3, 15
Single-model clusters	1; 2; 19; 20

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9104 atoms, of which 4548 are hydrogens and 0 are deuteriums.

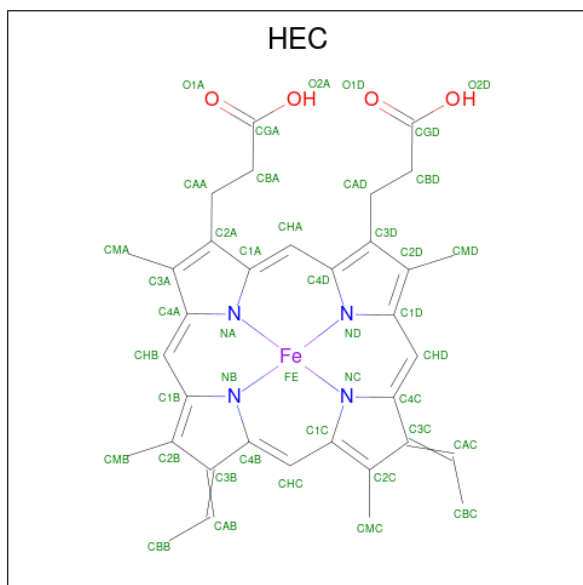
- Molecule 1 is a protein called Hemoglobin alpha subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2152	685	1083	187	194	3	
1	C	141	Total	C	H	N	O	S	0
			2152	685	1083	187	194	3	

- Molecule 2 is a protein called Hemoglobin beta subunit.

Mol	Chain	Residues	Atoms						Trace
2	B	146	Total	C	H	N	O	S	0
			2250	724	1127	195	201	3	
2	D	146	Total	C	H	N	O	S	0
			2250	724	1127	195	201	3	

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
3	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4
3	B	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4

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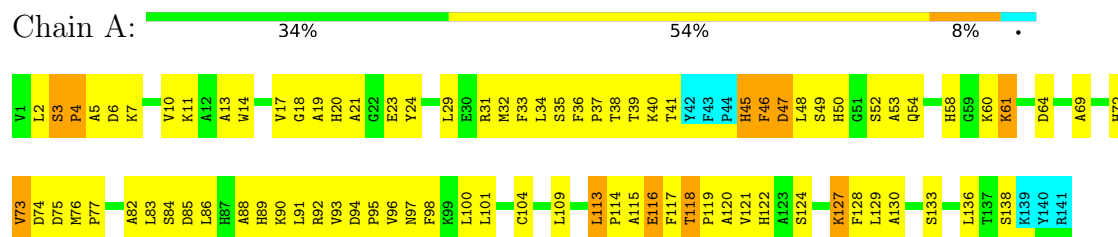
Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
3	C	1	75	34	1	32	4	4
3	D	1	75	34	1	32	4	4

4 Residue-property plots

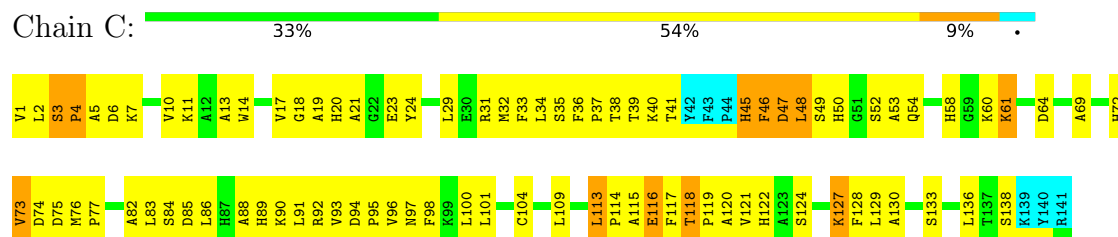
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

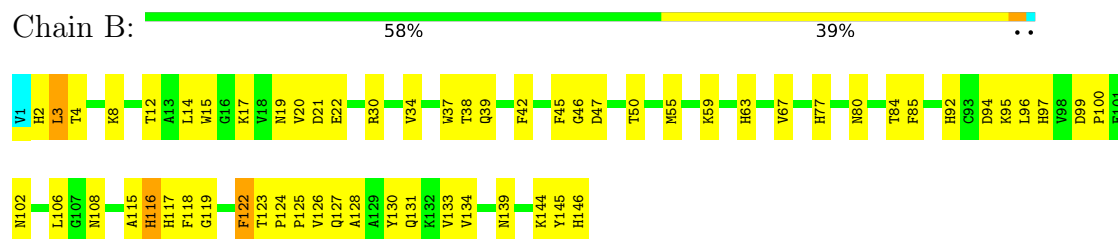
• Molecule 1: Hemoglobin alpha subunit



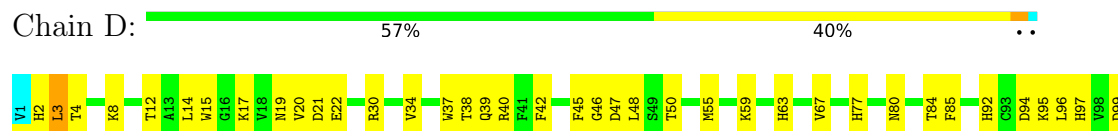
• Molecule 1: Hemoglobin alpha subunit



• Molecule 2: Hemoglobin beta subunit



• Molecule 2: Hemoglobin beta subunit





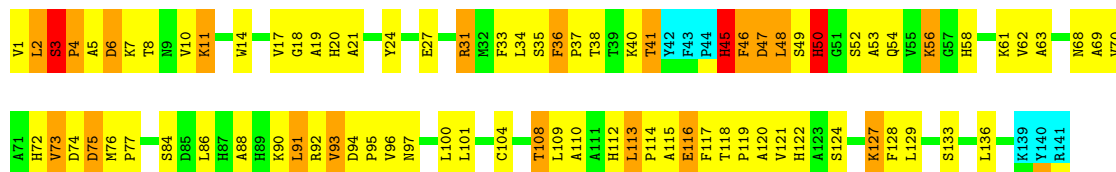
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

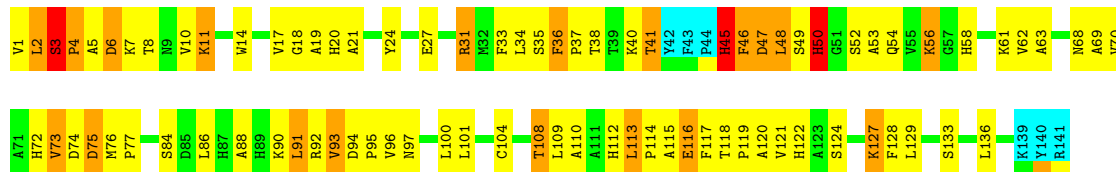
- Molecule 1: Hemoglobin alpha subunit

Chain A: 36% 44% 13% . .



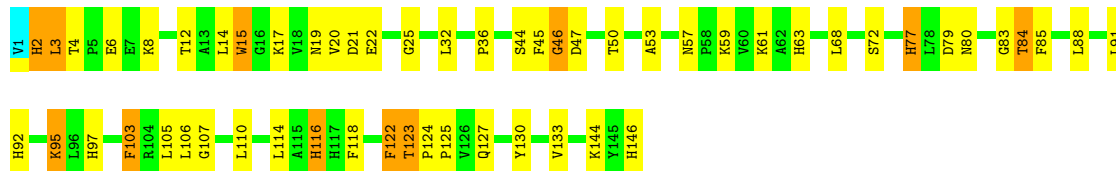
- Molecule 1: Hemoglobin alpha subunit

Chain C: 36% 44% 13% . .



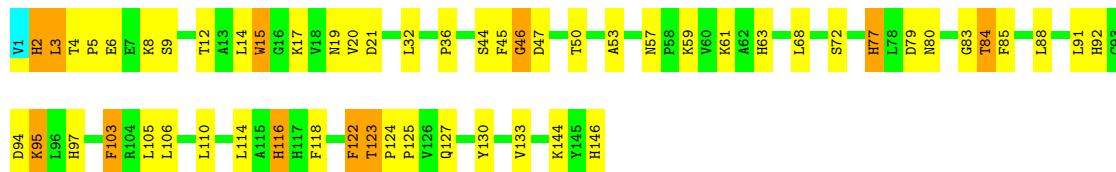
- Molecule 2: Hemoglobin beta subunit

Chain B: 61% 31% 8% .



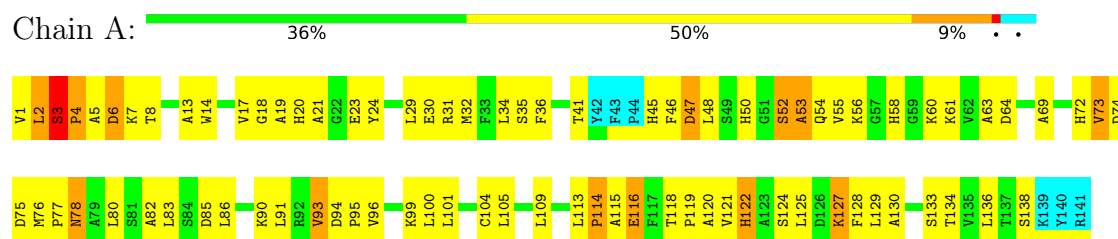
- Molecule 2: Hemoglobin beta subunit

Chain D: 61% 31% 8% .

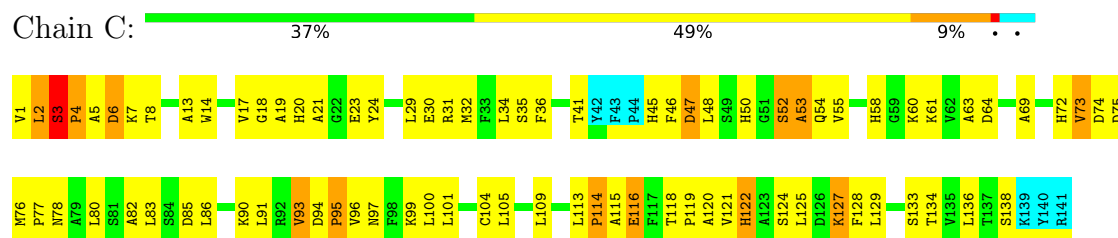


4.2.2 Score per residue for model 2

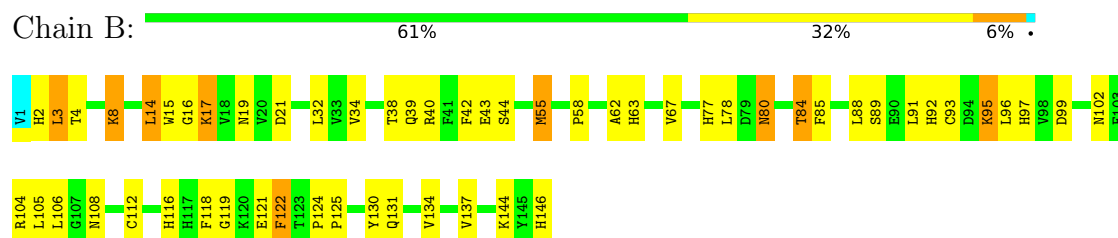
• Molecule 1: Hemoglobin alpha subunit



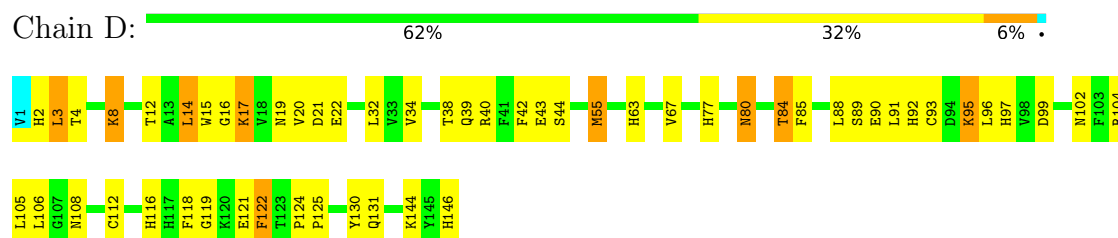
• Molecule 1: Hemoglobin alpha subunit



• Molecule 2: Hemoglobin beta subunit

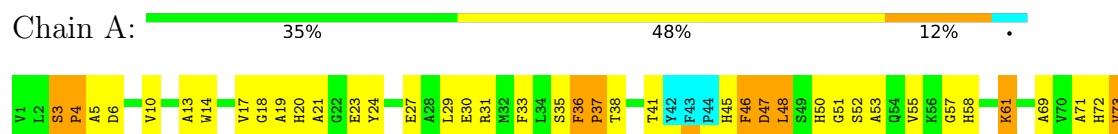


• Molecule 2: Hemoglobin beta subunit



4.2.3 Score per residue for model 3

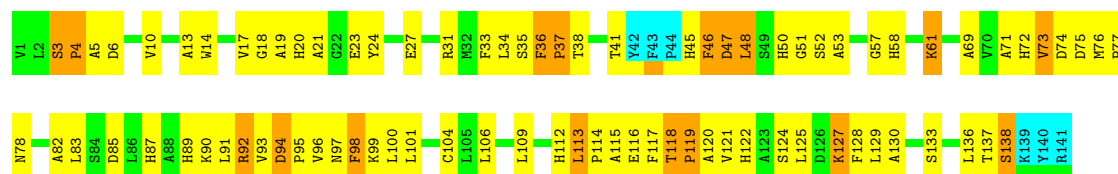
• Molecule 1: Hemoglobin alpha subunit





• Molecule 1: Hemoglobin alpha subunit

Chain C: 36% 48% 12% .



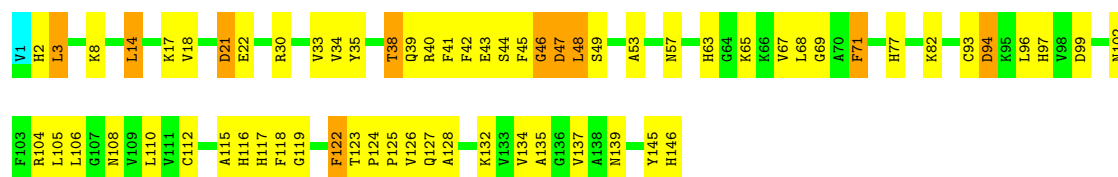
• Molecule 2: Hemoglobin beta subunit

Chain B: 53% 37% 9% .



• Molecule 2: Hemoglobin beta subunit

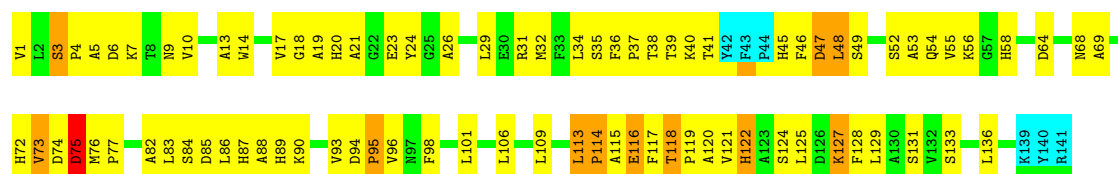
Chain D: 55% 38% 7% .



4.2.4 Score per residue for model 4

• Molecule 1: Hemoglobin alpha subunit

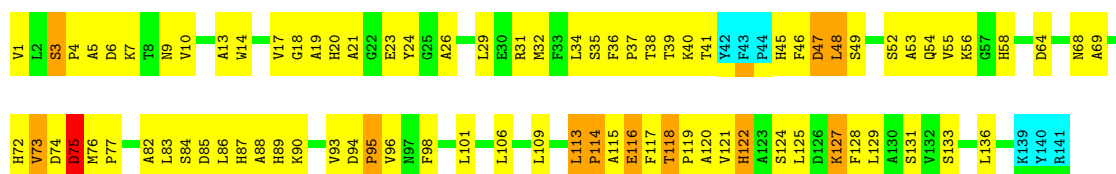
Chain A: 36% 51% 8% . .



• Molecule 1: Hemoglobin alpha subunit

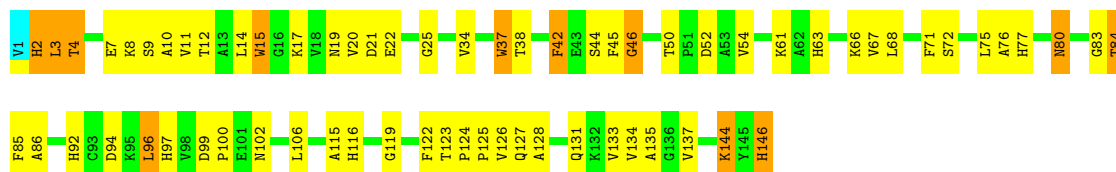
Chain C: 36% 51% 8% . .





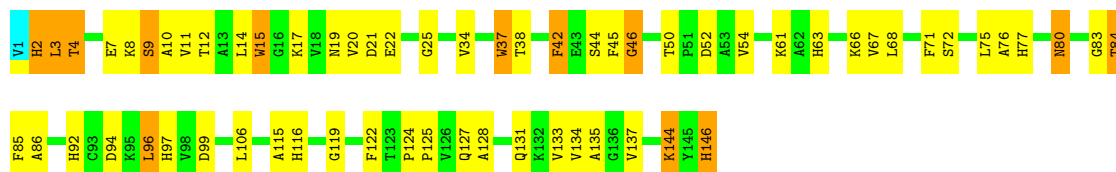
• Molecule 2: Hemoglobin beta subunit

Chain B: 53% 38% 8%



• Molecule 2: Hemoglobin beta subunit

Chain D: 56% 34% 9%



4.2.5 Score per residue for model 5 (medoid)

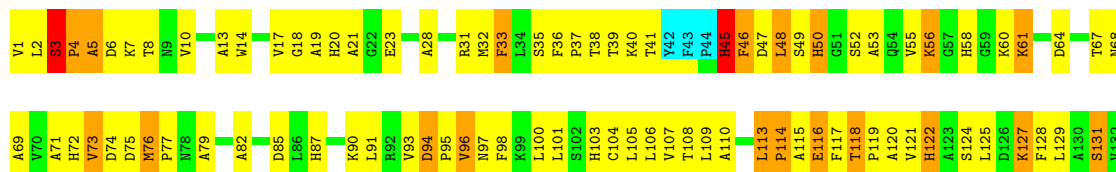
• Molecule 1: Hemoglobin alpha subunit

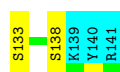
Chain A: 31% 50% 13%



• Molecule 1: Hemoglobin alpha subunit

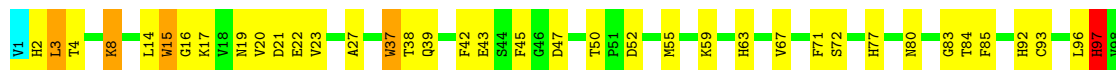
Chain C: 30% 50% 13%





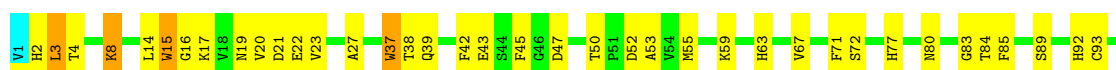
• Molecule 2: Hemoglobin beta subunit

Chain B: 55% 38% 5% ..



• Molecule 2: Hemoglobin beta subunit

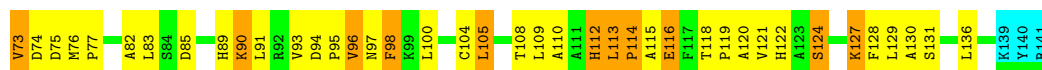
Chain D: 54% 39% 5% ..



4.2.6 Score per residue for model 6

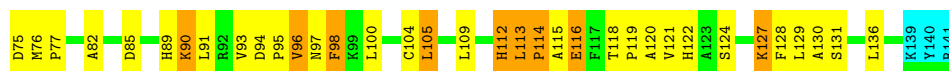
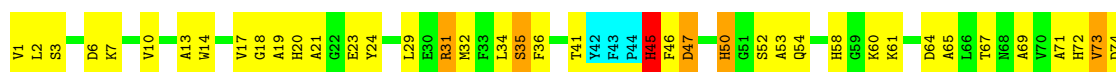
• Molecule 1: Hemoglobin alpha subunit

Chain A: 38% 46% 11% ..



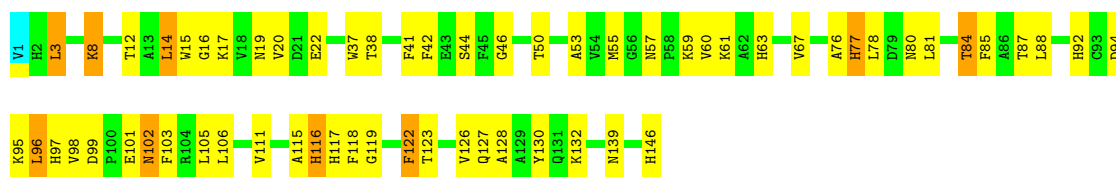
• Molecule 1: Hemoglobin alpha subunit

Chain C: 43% 43% 10% ..



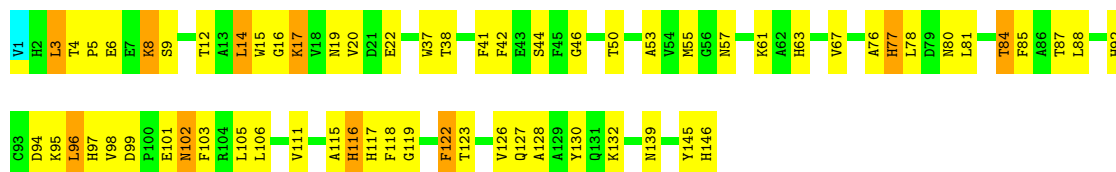
• Molecule 2: Hemoglobin beta subunit

Chain B: 58% 36% 6% ..



- Molecule 2: Hemoglobin beta subunit

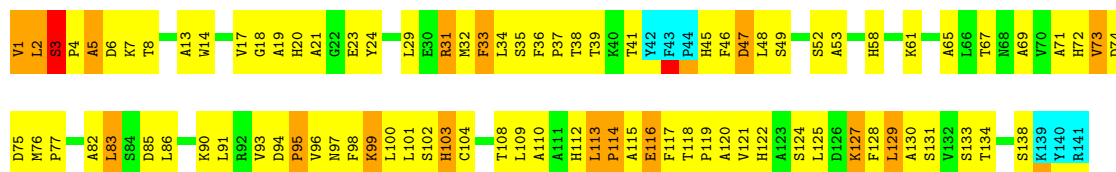
Chain D: 55% 37% 7%



4.2.7 Score per residue for model 7

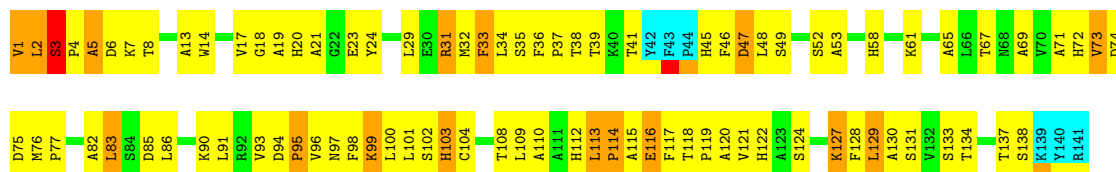
- Molecule 1: Hemoglobin alpha subunit

Chain A: 33% 51% 11%



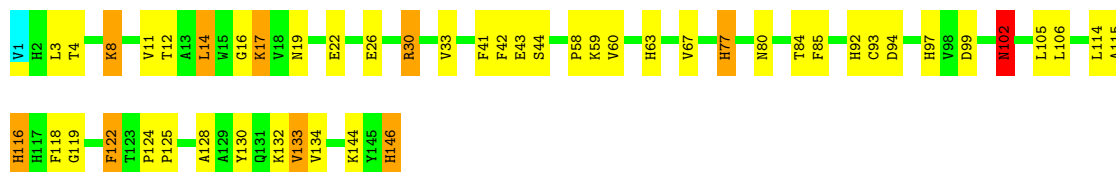
- Molecule 1: Hemoglobin alpha subunit

Chain C: 33% 51% 11%

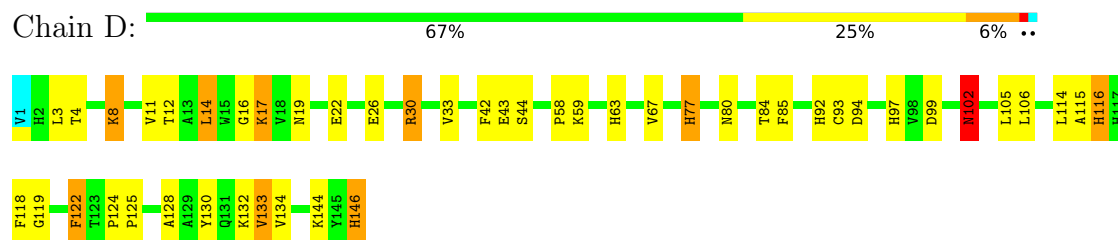


- Molecule 2: Hemoglobin beta subunit

Chain B: 66% 27% 6%

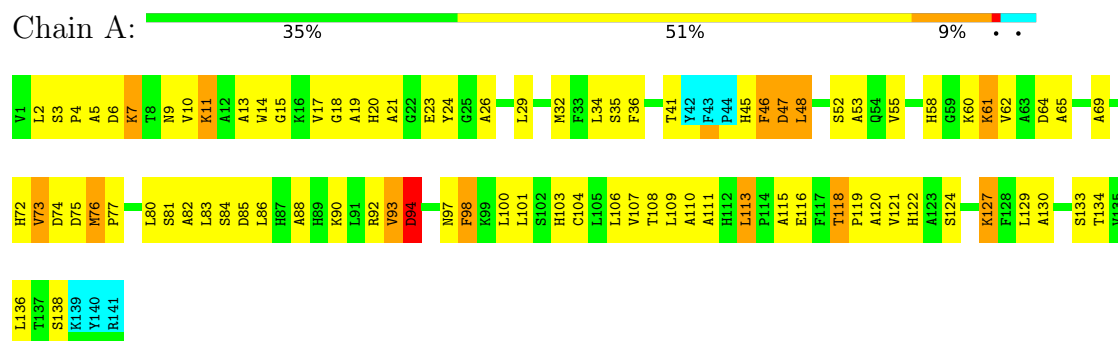


- Molecule 2: Hemoglobin beta subunit

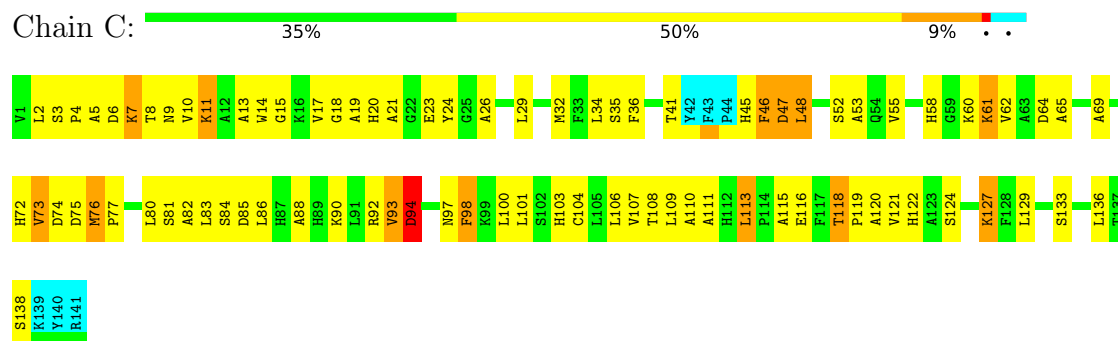


4.2.8 Score per residue for model 8

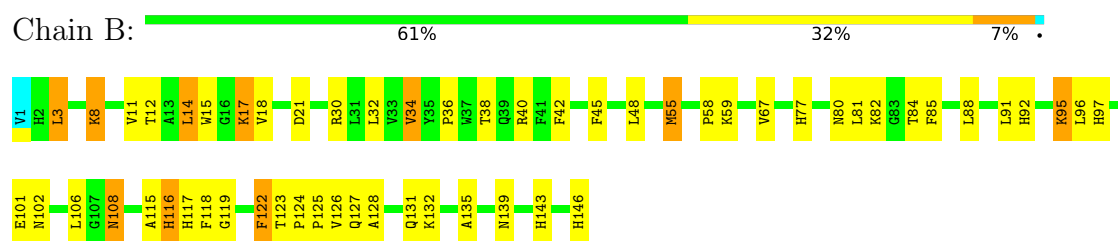
- Molecule 1: Hemoglobin alpha subunit



- Molecule 1: Hemoglobin alpha subunit

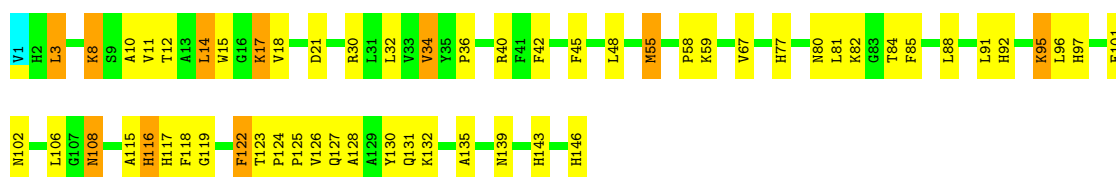


- Molecule 2: Hemoglobin beta subunit



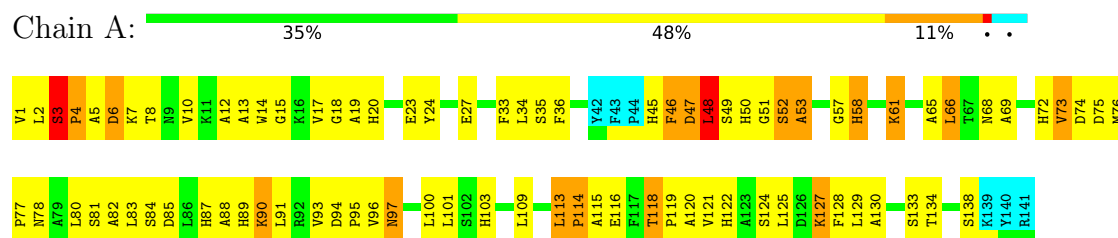
- Molecule 2: Hemoglobin beta subunit



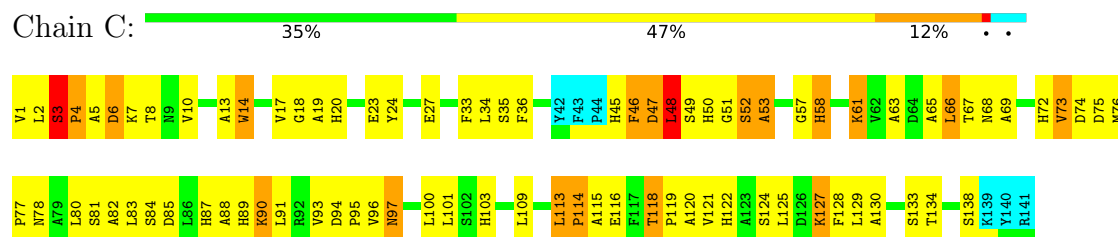


4.2.9 Score per residue for model 9

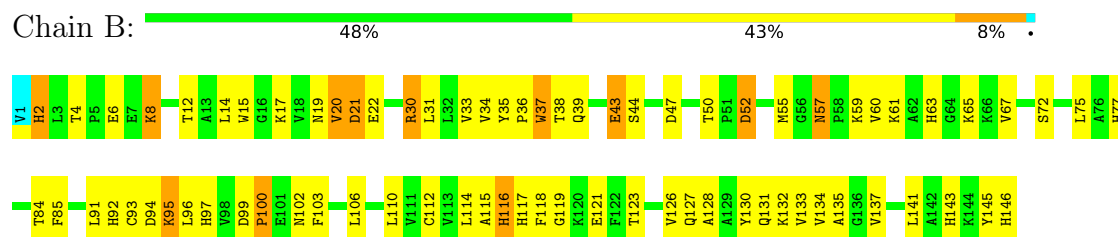
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit

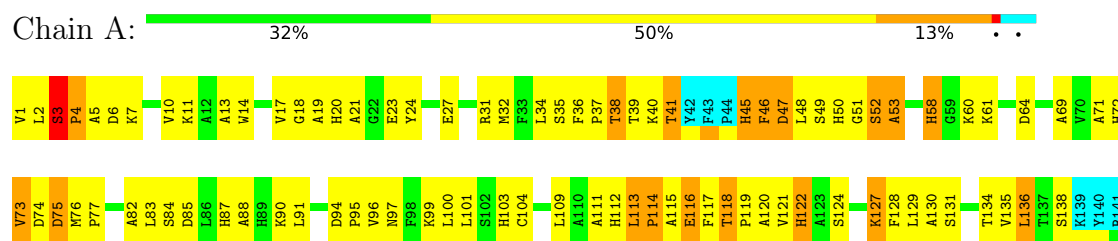


- Molecule 2: Hemoglobin beta subunit

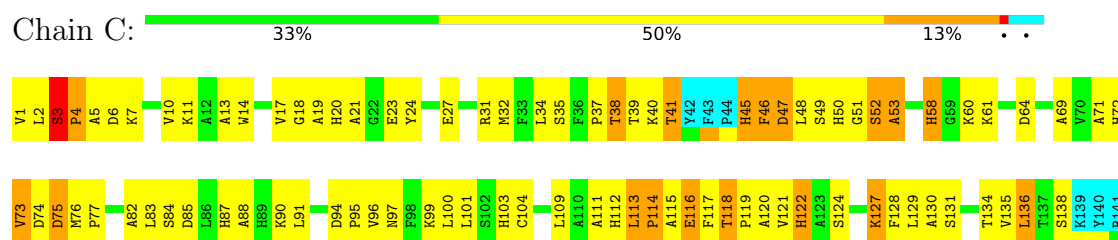


4.2.10 Score per residue for model 10

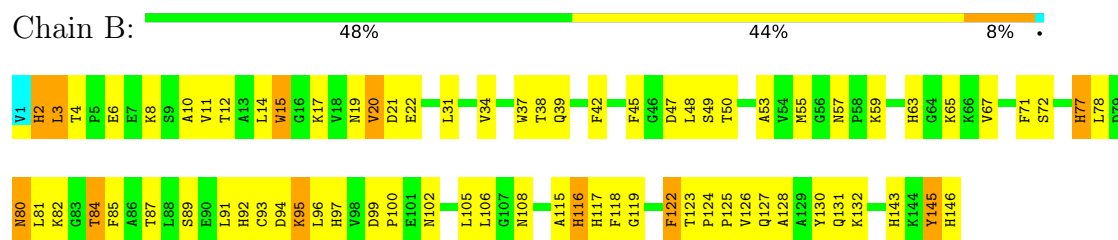
• Molecule 1: Hemoglobin alpha subunit



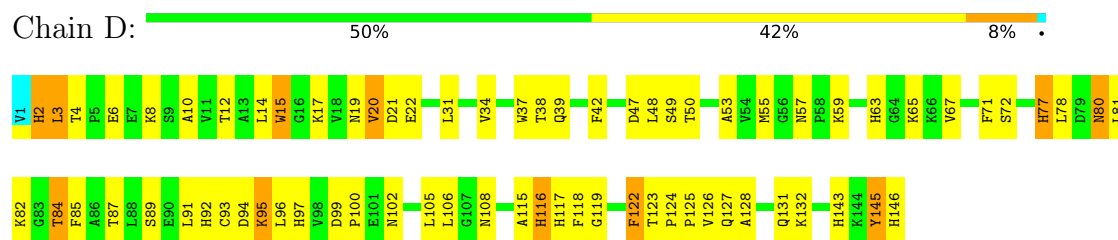
• Molecule 1: Hemoglobin alpha subunit



• Molecule 2: Hemoglobin beta subunit

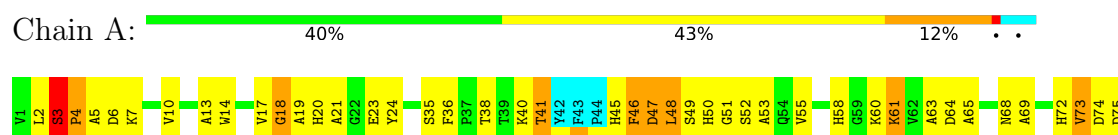


• Molecule 2: Hemoglobin beta subunit



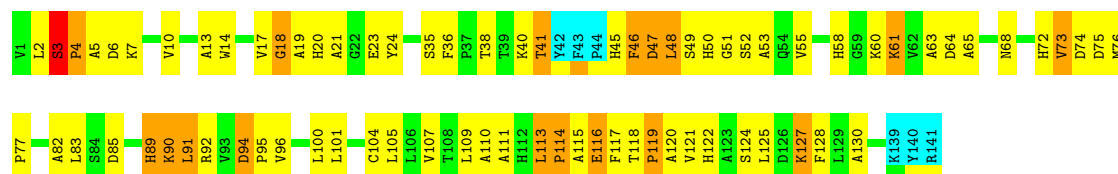
4.2.11 Score per residue for model 11

• Molecule 1: Hemoglobin alpha subunit

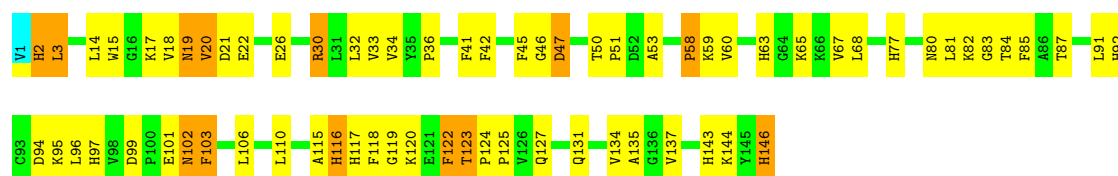




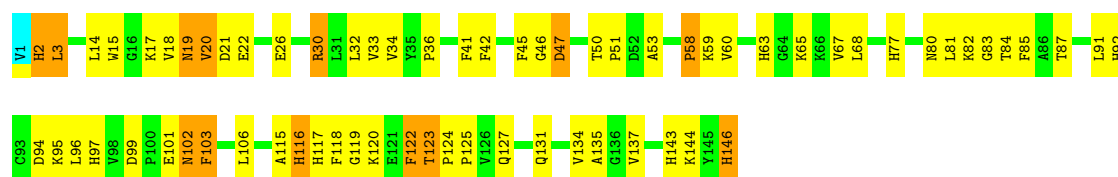
• Molecule 1: Hemoglobin alpha subunit



• Molecule 2: Hemoglobin beta subunit

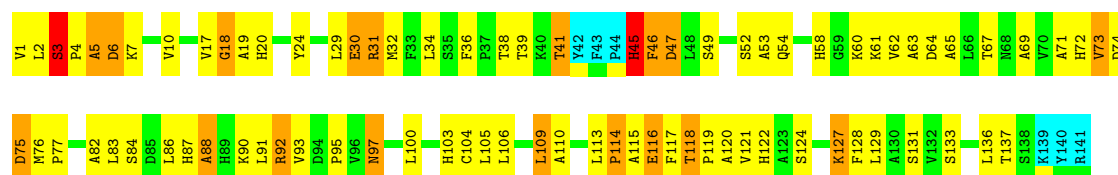


• Molecule 2: Hemoglobin beta subunit



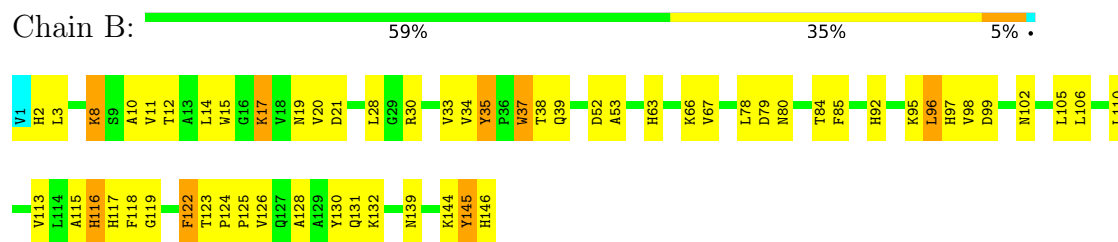
4.2.12 Score per residue for model 12

• Molecule 1: Hemoglobin alpha subunit

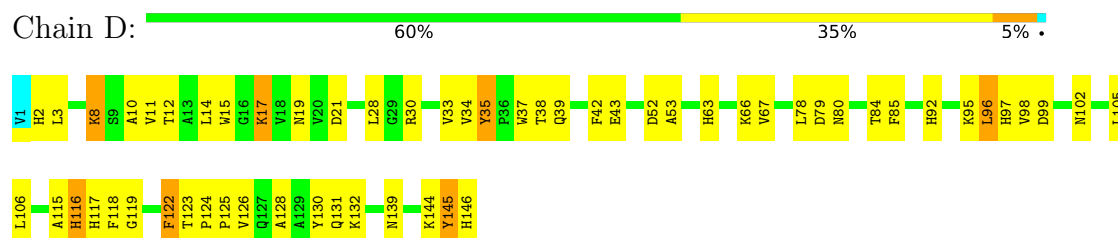


• Molecule 1: Hemoglobin alpha subunit



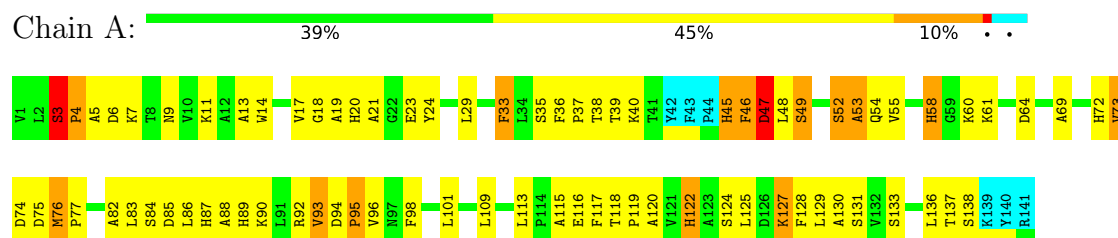


• Molecule 2: Hemoglobin beta subunit

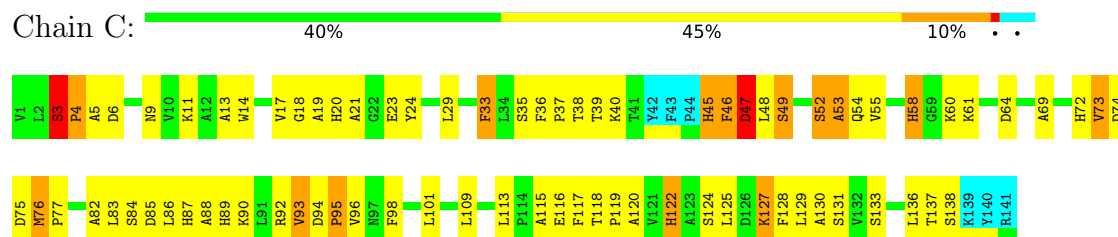


4.2.14 Score per residue for model 14

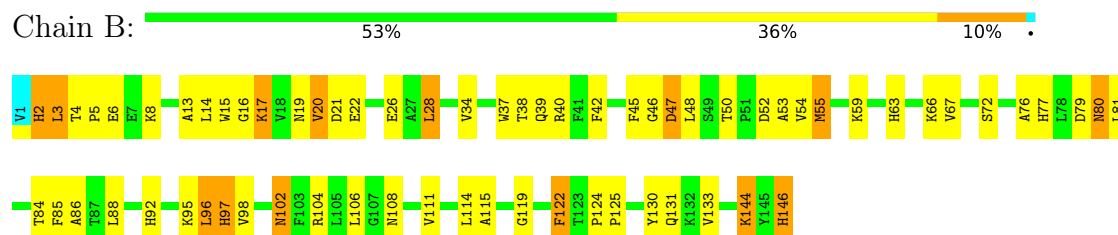
• Molecule 1: Hemoglobin alpha subunit



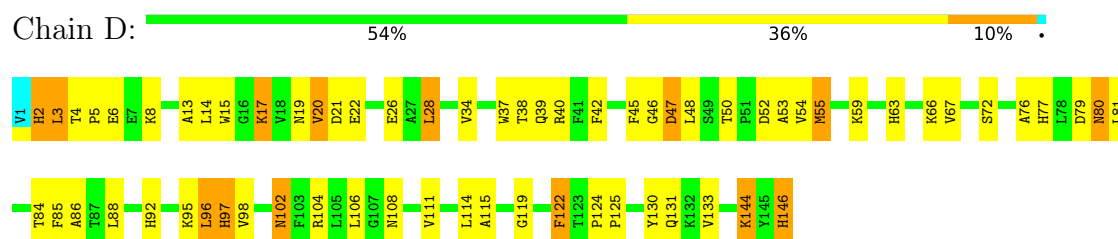
• Molecule 1: Hemoglobin alpha subunit



• Molecule 2: Hemoglobin beta subunit

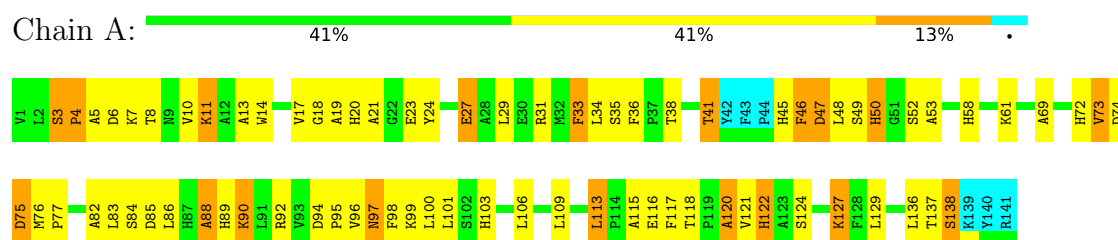


- Molecule 2: Hemoglobin beta subunit

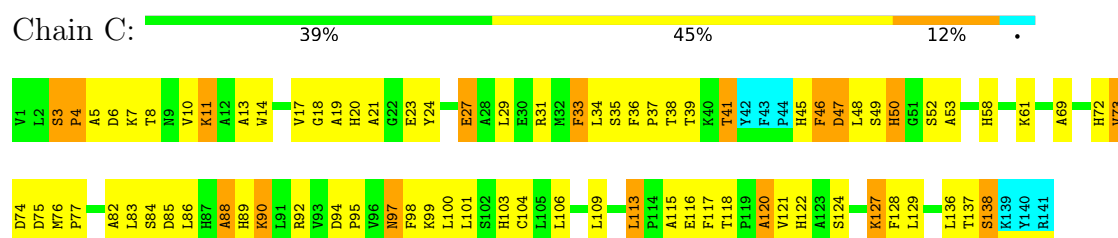


4.2.15 Score per residue for model 15

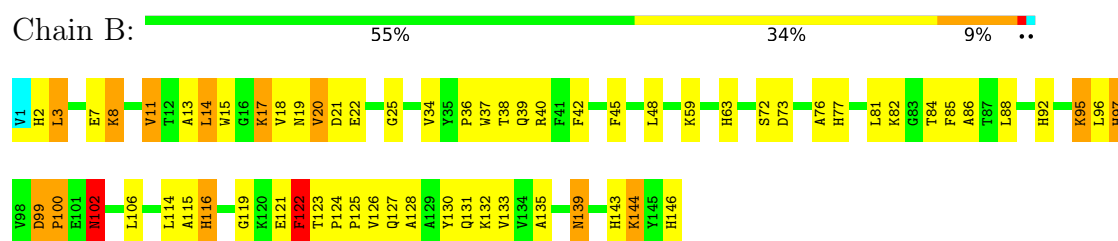
- Molecule 1: Hemoglobin alpha subunit



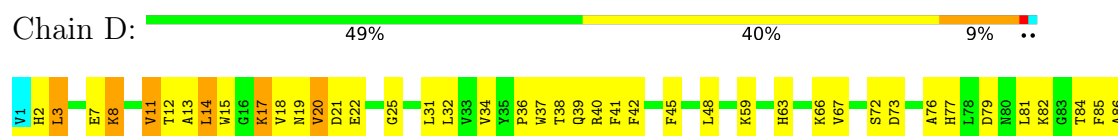
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit



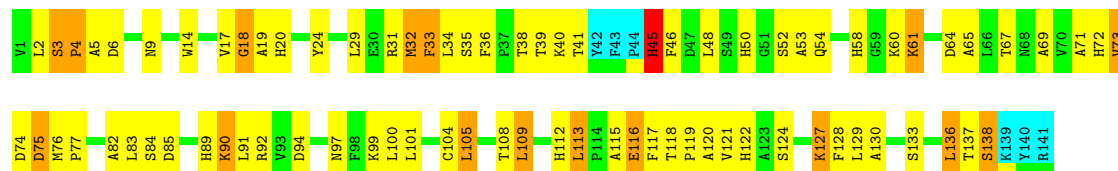
- Molecule 2: Hemoglobin beta subunit



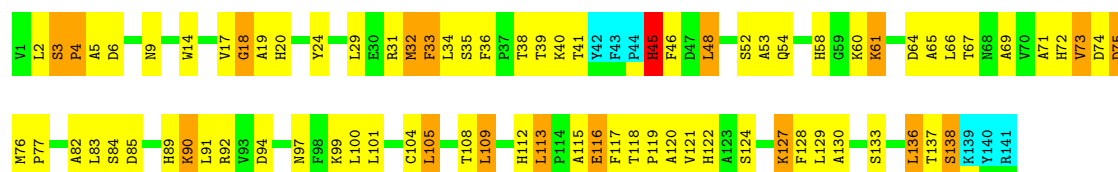


4.2.16 Score per residue for model 16

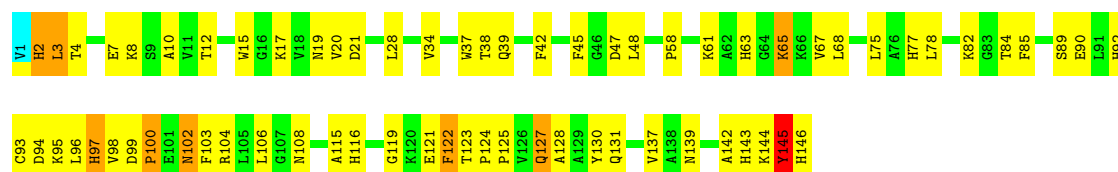
- Molecule 1: Hemoglobin alpha subunit



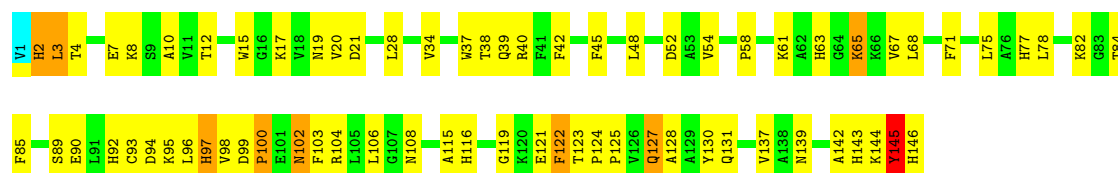
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit

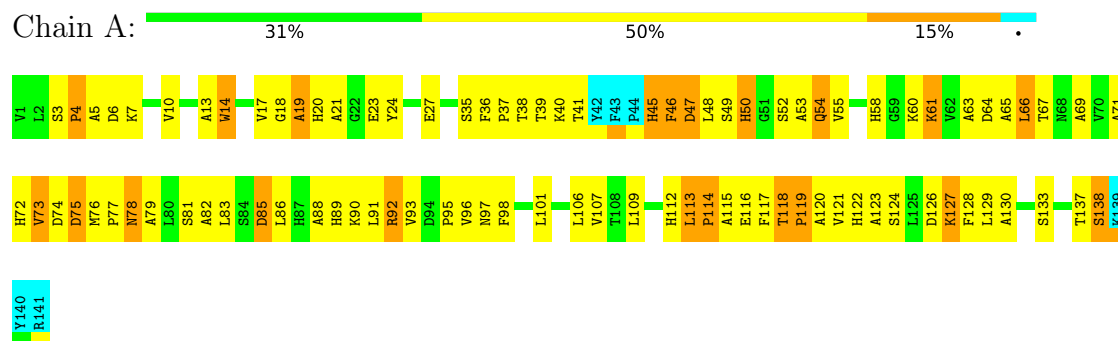


- Molecule 2: Hemoglobin beta subunit

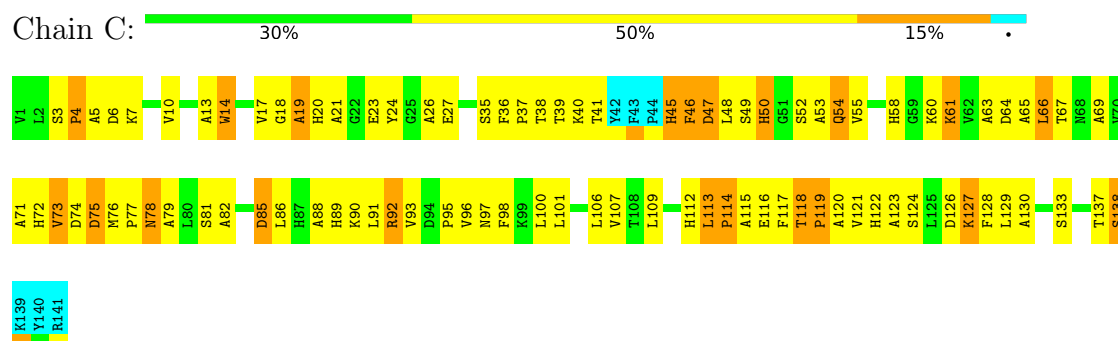


4.2.17 Score per residue for model 17

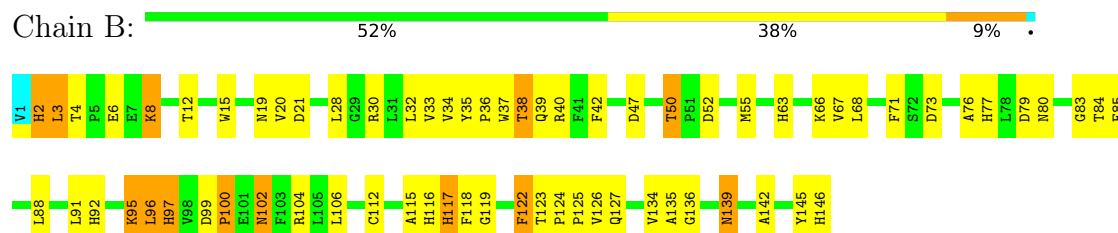
- Molecule 1: Hemoglobin alpha subunit



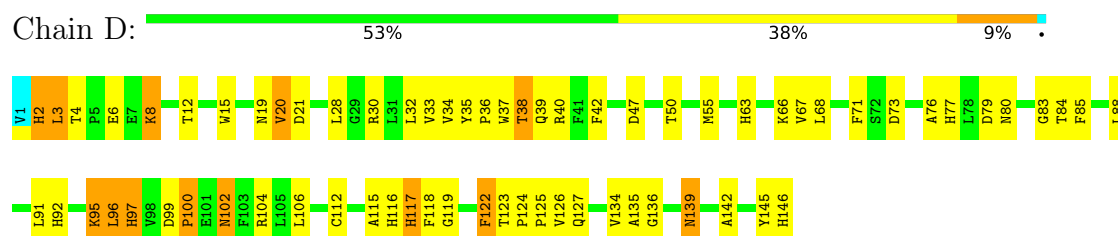
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit



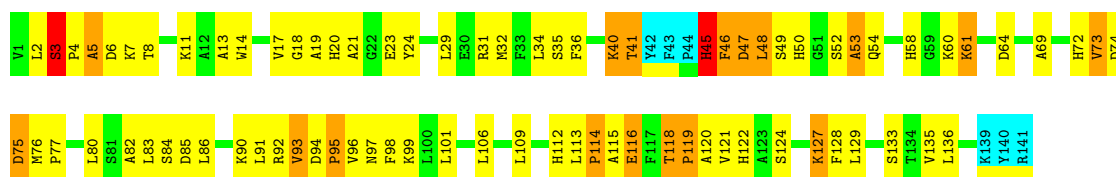
- Molecule 2: Hemoglobin beta subunit



4.2.18 Score per residue for model 18

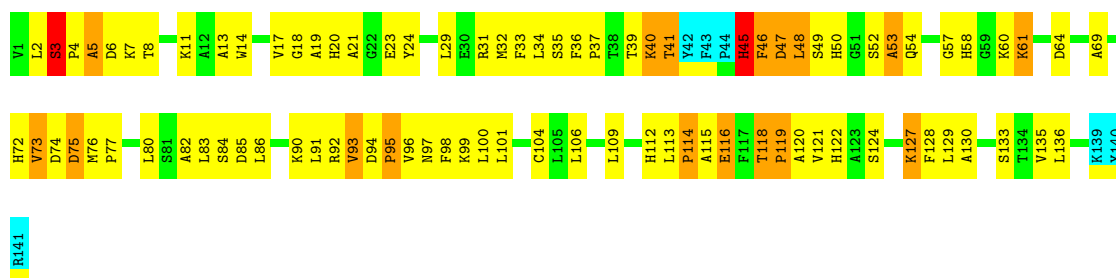
- Molecule 1: Hemoglobin alpha subunit





• Molecule 1: Hemoglobin alpha subunit

Chain C: 33% 49% 12% ..



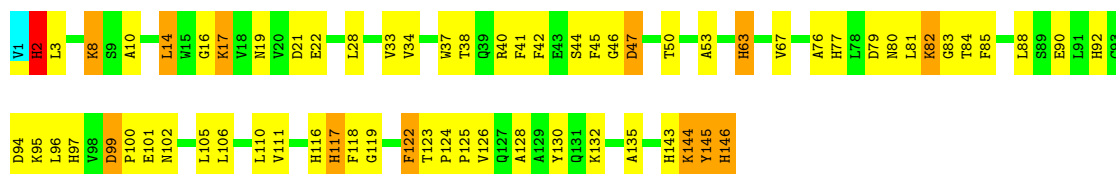
• Molecule 2: Hemoglobin beta subunit

Chain B: 52% 38% 8% ..



• Molecule 2: Hemoglobin beta subunit

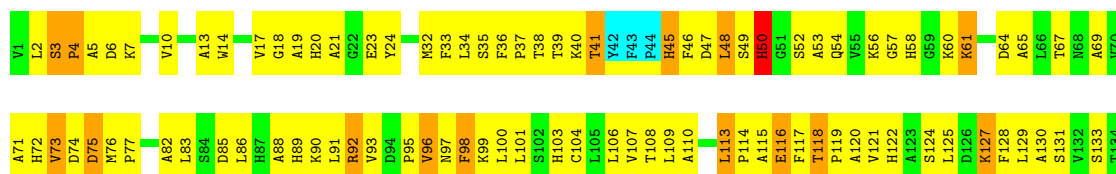
Chain D: 53% 37% 8% ..



4.2.19 Score per residue for model 19

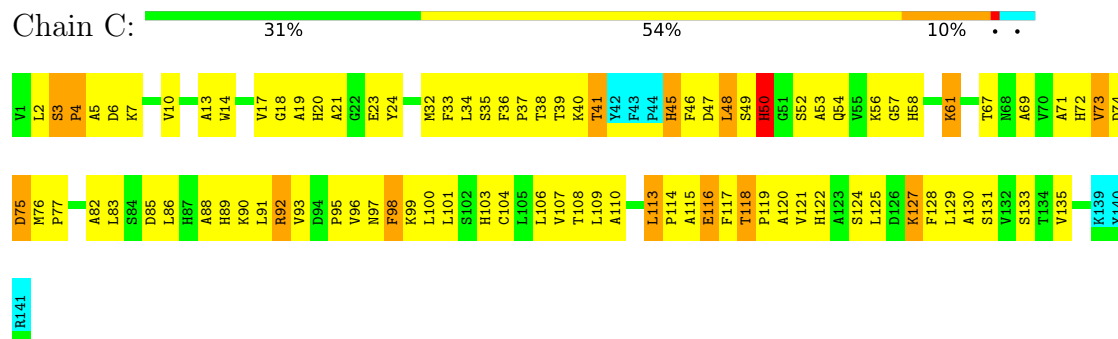
• Molecule 1: Hemoglobin alpha subunit

Chain A: 29% 55% 11% ..

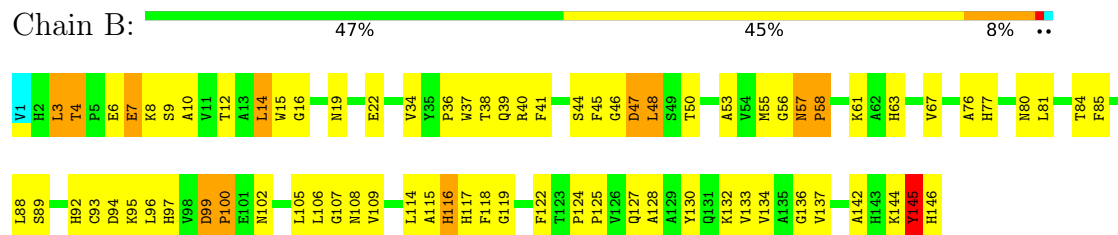




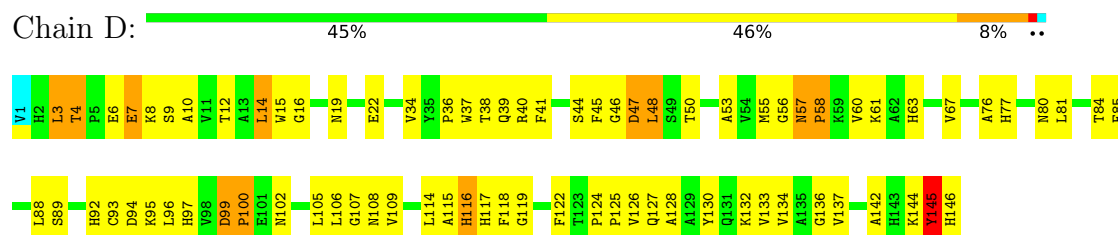
• Molecule 1: Hemoglobin alpha subunit



• Molecule 2: Hemoglobin beta subunit

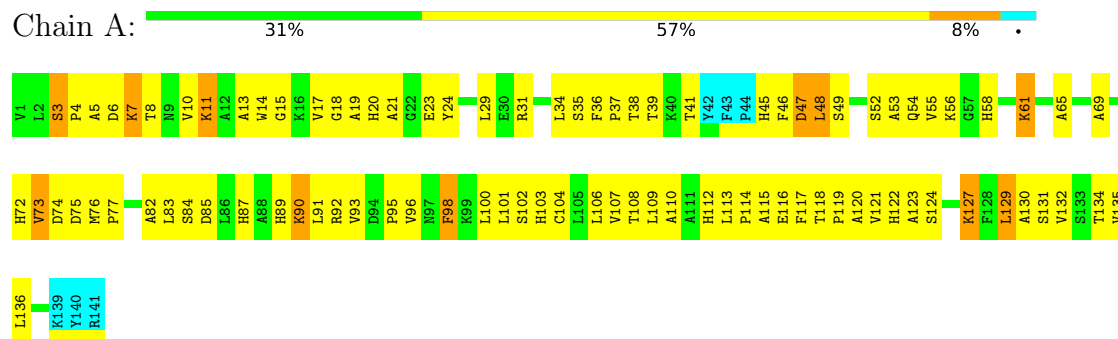


• Molecule 2: Hemoglobin beta subunit

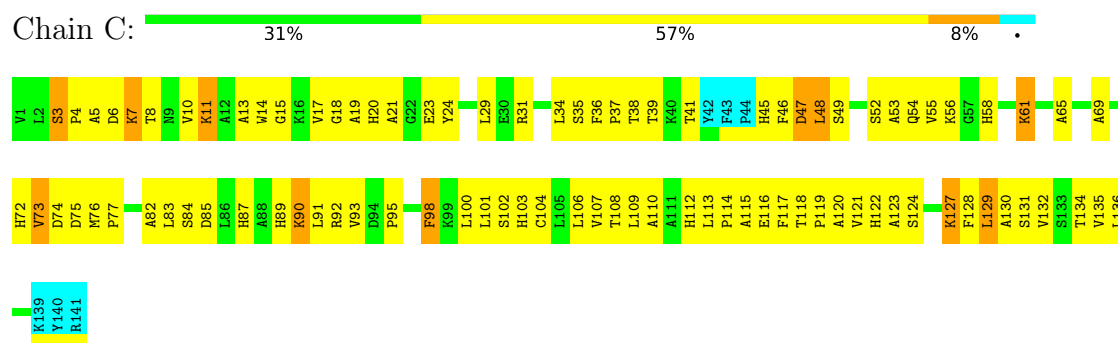


4.2.20 Score per residue for model 20

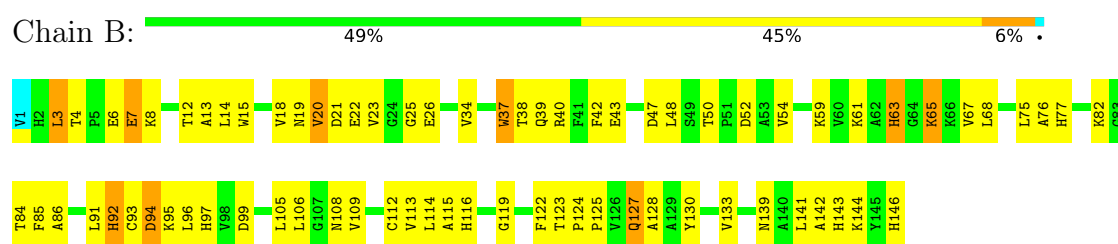
• Molecule 1: Hemoglobin alpha subunit



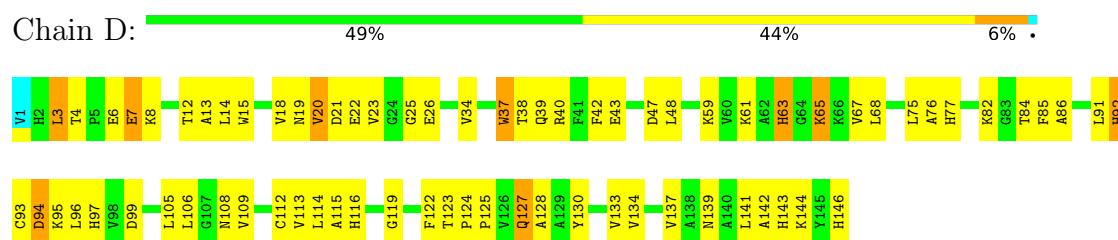
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit



- Molecule 2: Hemoglobin beta subunit



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with the least restraint violations, structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
xplor-nih	structure solution	2.14
xplor-nih	refinement	2.14

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1006	1023	1013	112±18
1	C	1006	1023	1013	112±22
2	B	1116	1116	1107	98±24
2	D	1116	1116	1107	102±28
3	A	43	32	32	10±5
3	B	43	32	32	23±11
3	C	43	32	32	13±11
3	D	43	32	32	23±14
All	All	88320	88120	87310	7771

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:40:ARG:CD	1:C:92:ARG:HD3	1.59	1.25	18	2
2:B:146:HIS:CD2	2:D:139:ASN:HD21	1.58	1.16	6	2
2:B:139:ASN:HD21	2:D:146:HIS:CD2	1.57	1.16	6	2
2:B:106:LEU:HD22	3:B:147:HEC:CBB	1.57	1.16	19	1
2:B:146:HIS:CD2	2:D:2:HIS:NE2	1.57	1.73	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:ARG:HD3	2:D:40:ARG:CD	1.57	1.19	18	2
2:D:106:LEU:CD2	3:D:147:HEC:HBB3	1.55	1.31	19	1
2:D:106:LEU:HD22	3:D:147:HEC:CBB	1.55	1.16	19	1
2:B:106:LEU:CD1	3:B:147:HEC:HAB	1.55	1.32	18	2
2:B:106:LEU:CD2	3:B:147:HEC:HBB3	1.54	1.31	19	1
2:B:2:HIS:NE2	2:D:146:HIS:CD2	1.52	1.77	15	1
1:A:101:LEU:HD22	3:A:142:HEC:CBB	1.52	1.35	15	2
1:A:41:THR:HG21	2:D:97:HIS:CD2	1.51	1.37	11	5
1:A:117:PHE:CZ	2:B:116:HIS:NE2	1.50	1.79	13	3
2:D:106:LEU:CD1	3:D:147:HEC:HAB	1.50	1.32	18	2
1:C:117:PHE:CZ	2:D:116:HIS:NE2	1.49	1.79	13	3
1:C:34:LEU:CD1	2:D:128:ALA:HB2	1.49	1.34	18	4
1:C:101:LEU:HD22	3:C:142:HEC:CBB	1.49	1.35	15	2
2:B:146:HIS:HD2	2:D:139:ASN:ND2	1.48	0.98	6	1
1:A:34:LEU:CD1	2:B:128:ALA:HB2	1.48	1.34	18	4
2:B:97:HIS:CD2	1:C:41:THR:HG21	1.47	1.44	11	5
2:D:67:VAL:HG13	3:D:147:HEC:C1B	1.46	1.41	19	11
2:B:139:ASN:ND2	2:D:146:HIS:HD2	1.46	0.98	6	1
1:A:92:ARG:CG	2:D:40:ARG:NH2	1.46	1.79	16	1
1:C:48:LEU:HD11	3:C:142:HEC:CHA	1.45	1.41	12	1
1:A:92:ARG:CD	2:D:40:ARG:NH2	1.45	1.69	16	1
2:B:67:VAL:HG13	3:B:147:HEC:C1B	1.45	1.41	19	12
2:B:42:PHE:CZ	3:B:147:HEC:CBC	1.42	2.02	17	4
1:A:92:ARG:NE	2:D:40:ARG:HB2	1.40	1.30	19	1
2:D:42:PHE:CZ	3:D:147:HEC:CBC	1.40	2.02	17	3
1:C:34:LEU:HD12	2:D:128:ALA:CB	1.40	1.45	18	1
1:A:92:ARG:HD3	2:D:40:ARG:NE	1.39	1.27	16	2
1:A:34:LEU:HD12	2:B:128:ALA:CB	1.39	1.45	18	1
2:D:42:PHE:HB3	3:D:147:HEC:CMA	1.36	1.49	12	1
2:D:38:THR:C	3:D:147:HEC:C1C	1.35	1.93	12	1
3:B:147:HEC:CHC	2:D:106:LEU:CD1	1.35	2.02	15	1
1:A:92:ARG:NH2	2:D:40:ARG:HE	1.35	1.17	15	1
1:A:92:ARG:CD	2:D:40:ARG:HD2	1.35	1.49	18	2
1:A:41:THR:HG21	2:D:97:HIS:ND1	1.33	1.31	17	2
2:B:40:ARG:HB2	1:C:92:ARG:NE	1.33	1.35	19	1
2:B:146:HIS:CD2	2:D:139:ASN:ND2	1.31	1.80	6	2
1:A:96:VAL:HG11	2:D:99:ASP:OD2	1.31	1.24	11	1
2:B:97:HIS:ND1	1:C:41:THR:HG21	1.31	1.37	17	2
1:A:92:ARG:NH2	2:D:40:ARG:NE	1.31	1.78	15	1
2:B:40:ARG:HE	1:C:92:ARG:NH2	1.31	1.21	15	1
2:D:42:PHE:O	3:D:147:HEC:HMA2	1.31	1.13	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:139:ASN:ND2	2:D:146:HIS:CD2	1.30	1.82	6	2
2:B:40:ARG:HD2	1:C:92:ARG:CD	1.30	1.55	18	2
2:B:82:LYS:NZ	2:D:82:LYS:HZ1	1.28	1.23	15	1
2:D:42:PHE:CB	3:D:147:HEC:CMA	1.28	2.10	12	1
1:A:92:ARG:NE	2:D:40:ARG:CB	1.28	1.97	19	1
2:B:82:LYS:NZ	2:D:82:LYS:NZ	1.27	1.81	15	1
2:D:32:LEU:O	3:D:147:HEC:HMB1	1.27	1.09	15	1
2:D:63:HIS:NE2	3:D:147:HEC:CHA	1.26	1.99	16	8
1:A:92:ARG:NH2	3:D:147:HEC:HBD2	1.26	1.43	12	1
2:B:40:ARG:CB	1:C:92:ARG:NE	1.25	1.99	19	1
2:B:99:ASP:OD2	1:C:96:VAL:HG11	1.25	1.24	11	1
1:A:41:THR:CG2	2:D:97:HIS:CE1	1.25	2.10	17	3
2:B:40:ARG:NE	1:C:92:ARG:NH2	1.25	1.85	15	1
2:D:42:PHE:CZ	3:D:147:HEC:HBC3	1.25	1.64	17	5
2:B:40:ARG:CZ	1:C:92:ARG:CB	1.24	2.15	17	2
1:A:38:THR:HG22	2:D:97:HIS:ND1	1.24	1.48	7	1
1:A:111:ALA:HB2	2:B:122:PHE:CE2	1.24	1.67	8	3
2:D:38:THR:N	3:D:147:HEC:CHC	1.23	1.74	12	1
2:B:97:HIS:CE1	1:C:41:THR:HG21	1.23	1.63	17	3
2:B:63:HIS:NE2	3:B:147:HEC:CHA	1.23	1.99	16	9
1:A:101:LEU:CD2	3:A:142:HEC:CBB	1.23	2.17	15	4
1:C:111:ALA:HB2	2:D:122:PHE:CE2	1.23	1.67	8	3
1:A:92:ARG:CD	2:D:40:ARG:CD	1.23	2.09	18	1
2:D:38:THR:N	3:D:147:HEC:HHC	1.22	1.27	12	1
2:B:146:HIS:CE1	2:D:139:ASN:OD1	1.22	1.92	8	1
2:B:42:PHE:CE1	3:B:147:HEC:HBC1	1.22	1.68	17	2
1:A:96:VAL:HG21	2:D:99:ASP:CB	1.22	1.63	18	2
2:B:40:ARG:CD	1:C:92:ARG:CD	1.22	2.15	18	1
1:A:41:THR:HG21	2:D:97:HIS:CE1	1.21	1.58	17	2
2:B:40:ARG:NH1	1:C:92:ARG:HB3	1.21	1.49	17	1
1:C:101:LEU:CD2	3:C:142:HEC:CBB	1.21	2.17	15	4
2:D:42:PHE:CE1	3:D:147:HEC:HBC1	1.21	1.68	17	1
1:A:117:PHE:CD1	2:B:30:ARG:NH2	1.21	2.08	3	3
1:A:117:PHE:CZ	2:B:116:HIS:CD2	1.21	2.28	13	1
1:A:92:ARG:CB	2:D:40:ARG:CZ	1.21	2.17	17	2
2:D:38:THR:CA	3:D:147:HEC:CHC	1.21	2.09	12	1
2:D:42:PHE:CB	3:D:147:HEC:HMA1	1.20	1.65	12	1
1:A:96:VAL:CG1	2:D:99:ASP:OD2	1.20	1.89	11	1
1:C:101:LEU:CD2	3:C:142:HEC:HBB3	1.20	1.67	15	7
2:D:42:PHE:CE2	3:D:147:HEC:HMD3	1.20	1.72	2	1
1:C:117:PHE:CD1	2:D:30:ARG:NH2	1.19	2.08	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:117:PHE:CZ	2:D:116:HIS:CD2	1.19	2.28	13	1
1:A:41:THR:HG21	2:D:97:HIS:CG	1.19	1.71	12	4
1:A:101:LEU:CD2	3:A:142:HEC:HBB3	1.18	1.67	15	7
2:B:106:LEU:HD21	3:B:147:HEC:CHC	1.18	1.67	2	1
1:C:45:HIS:N	3:C:142:HEC:HMA2	1.18	1.22	12	1
2:D:106:LEU:HD21	3:D:147:HEC:CHC	1.18	1.66	2	1
2:B:99:ASP:OD2	1:C:96:VAL:CG1	1.18	1.92	11	1
1:A:92:ARG:HB3	2:D:40:ARG:NH1	1.18	1.50	17	1
2:B:42:PHE:CE2	3:B:147:HEC:HMD3	1.18	1.72	2	1
1:A:92:ARG:HH21	2:D:40:ARG:NE	1.18	1.31	15	1
2:D:39:GLN:N	3:D:147:HEC:C4B	1.18	1.94	12	1
1:C:32:MET:HE2	3:C:142:HEC:CAB	1.17	1.70	12	1
1:A:92:ARG:HD3	2:D:40:ARG:CZ	1.17	1.62	16	1
2:B:99:ASP:CB	1:C:96:VAL:HG21	1.17	1.69	18	1
2:B:139:ASN:OD1	2:D:146:HIS:CE1	1.17	1.95	8	1
2:B:106:LEU:CD2	3:B:147:HEC:HHC	1.17	1.69	2	1
2:D:106:LEU:CD1	3:D:147:HEC:CHC	1.17	2.23	9	13
2:D:106:LEU:CD2	3:D:147:HEC:HHC	1.16	1.69	2	1
1:C:32:MET:CE	3:C:142:HEC:HAB	1.16	1.67	12	1
2:B:42:PHE:CZ	3:B:147:HEC:HBC3	1.16	1.64	17	6
2:B:97:HIS:ND1	1:C:38:THR:HG22	1.16	1.53	7	1
2:D:106:LEU:CG	3:D:147:HEC:CAB	1.16	2.24	18	1
2:B:97:HIS:CE1	1:C:41:THR:CG2	1.15	2.16	17	3
2:D:42:PHE:HB2	3:D:147:HEC:C4A	1.15	1.69	12	1
2:B:106:LEU:CD1	3:B:147:HEC:CHC	1.15	2.23	9	14
2:B:97:HIS:CG	1:C:41:THR:HG21	1.15	1.75	12	3
1:C:48:LEU:CD1	3:C:142:HEC:CHA	1.15	2.22	12	1
2:B:106:LEU:CG	3:B:147:HEC:CAB	1.15	2.24	18	1
2:B:2:HIS:NE2	2:D:146:HIS:HD2	1.15	1.16	15	1
1:A:96:VAL:HG11	2:D:99:ASP:CG	1.15	1.60	11	1
2:D:32:LEU:O	3:D:147:HEC:CMB	1.15	1.93	15	1
2:D:42:PHE:HB2	3:D:147:HEC:CHB	1.14	1.72	12	1
3:B:147:HEC:CHC	2:D:106:LEU:HD13	1.14	1.60	15	1
2:B:82:LYS:HZ1	2:D:82:LYS:NZ	1.14	1.34	15	1
2:B:42:PHE:HZ	3:B:147:HEC:CBC	1.14	1.41	17	2
1:C:117:PHE:HZ	2:D:116:HIS:NE2	1.13	1.21	13	1
2:B:106:LEU:CD1	3:B:147:HEC:CAB	1.13	2.26	18	2
2:D:106:LEU:HD12	3:D:147:HEC:CAB	1.13	1.72	18	1
2:D:42:PHE:HZ	3:D:147:HEC:CBC	1.13	1.41	17	1
2:D:106:LEU:CG	3:D:147:HEC:HAB	1.13	1.72	18	1
2:D:106:LEU:CD1	3:D:147:HEC:CAB	1.12	2.26	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:146:HIS:HD2	2:D:2:HIS:NE2	1.12	1.15	15	1
3:B:147:HEC:HHC	2:D:106:LEU:CD1	1.12	1.74	15	1
1:A:92:ARG:HH22	3:D:147:HEC:CBD	1.12	1.55	12	1
2:B:106:LEU:HD12	3:B:147:HEC:CAB	1.12	1.72	18	1
2:D:38:THR:C	3:D:147:HEC:CHC	1.12	2.17	12	1
2:B:106:LEU:CG	3:B:147:HEC:HAB	1.12	1.72	18	1
1:A:41:THR:CG2	2:D:97:HIS:CD2	1.12	2.33	11	3
1:A:92:ARG:HG3	2:D:40:ARG:NH2	1.12	1.45	16	1
2:D:106:LEU:CD2	3:D:147:HEC:CHC	1.11	2.27	2	1
2:D:106:LEU:HD22	3:D:147:HEC:HAB	1.11	1.17	10	12
1:C:101:LEU:HD13	3:C:142:HEC:CHC	1.11	1.75	15	5
1:C:48:LEU:HD11	3:C:142:HEC:C1A	1.11	1.75	12	1
1:A:101:LEU:HD13	3:A:142:HEC:CHC	1.11	1.75	15	5
2:D:63:HIS:NE2	3:D:147:HEC:HAD2	1.11	1.59	19	4
2:B:63:HIS:NE2	3:B:147:HEC:HAD2	1.11	1.59	19	4
2:B:99:ASP:CG	1:C:96:VAL:HG11	1.11	1.65	11	1
1:C:101:LEU:CD1	3:C:142:HEC:CHC	1.11	2.29	19	5
2:B:146:HIS:NE2	2:D:139:ASN:ND2	1.10	1.99	8	2
1:A:92:ARG:CZ	2:D:40:ARG:HB2	1.10	1.77	19	1
2:B:67:VAL:HG13	3:B:147:HEC:C2B	1.10	1.76	9	17
2:B:139:ASN:ND2	2:D:146:HIS:NE2	1.10	1.99	8	2
2:D:106:LEU:HD21	3:D:147:HEC:HHC	1.10	1.16	2	1
2:B:42:PHE:CE1	3:B:147:HEC:CBC	1.10	2.33	12	3
2:D:67:VAL:HG13	3:D:147:HEC:C2B	1.09	1.76	9	16
2:B:40:ARG:HB2	1:C:92:ARG:CZ	1.09	1.76	19	1
1:C:117:PHE:CE1	2:D:30:ARG:NH2	1.08	2.21	3	2
1:A:101:LEU:CD1	3:A:142:HEC:CHC	1.08	2.29	19	5
2:D:67:VAL:HG22	3:D:147:HEC:C1B	1.08	1.77	9	12
1:A:117:PHE:CE1	2:B:30:ARG:NH2	1.08	2.21	3	2
1:A:96:VAL:HG21	2:D:99:ASP:HB3	1.08	1.21	18	2
2:D:63:HIS:CE1	3:D:147:HEC:CHA	1.08	2.36	2	13
1:A:94:ASP:OD1	2:D:40:ARG:NH1	1.08	1.87	3	1
1:A:92:ARG:CD	2:D:40:ARG:CZ	1.08	2.20	16	2
2:B:63:HIS:CE1	3:B:147:HEC:CHA	1.08	2.36	2	14
2:B:67:VAL:HG22	3:B:147:HEC:C1B	1.07	1.77	9	13
1:C:45:HIS:N	3:C:142:HEC:CMA	1.07	2.17	12	1
2:B:139:ASN:ND2	2:D:139:ASN:ND2	1.07	2.01	3	1
2:B:40:ARG:CZ	1:C:92:ARG:HB2	1.07	1.78	17	2
2:B:146:HIS:O	2:D:132:LYS:HD3	1.06	1.50	15	1
2:B:67:VAL:HG22	3:B:147:HEC:CHB	1.06	1.80	9	13
1:C:31:ARG:NH1	2:D:127:GLN:CG	1.06	2.19	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:86:LEU:HD11	3:C:142:HEC:HBD2	1.06	1.13	7	2
2:B:135:ALA:O	2:D:146:HIS:CD2	1.06	2.08	17	1
2:B:106:LEU:CD2	3:B:147:HEC:CHC	1.06	2.27	2	1
2:B:40:ARG:NE	1:C:92:ARG:HH21	1.06	1.39	15	1
2:D:106:LEU:HD12	3:D:147:HEC:CHC	1.05	1.81	9	6
1:A:31:ARG:NH1	2:B:127:GLN:CG	1.05	2.18	16	2
2:B:97:HIS:CD2	1:C:41:THR:CG2	1.05	2.40	11	3
1:A:92:ARG:HB3	2:D:40:ARG:CZ	1.05	1.76	17	1
2:D:67:VAL:HG22	3:D:147:HEC:CHB	1.05	1.80	9	12
2:D:42:PHE:O	3:D:147:HEC:CMA	1.05	2.04	12	1
2:B:106:LEU:HD22	3:B:147:HEC:HAB	1.04	1.17	10	13
2:D:42:PHE:HE2	3:D:147:HEC:HMD3	1.04	1.01	2	1
2:D:42:PHE:C	3:D:147:HEC:HMA2	1.04	1.71	12	1
2:D:42:PHE:CE1	3:D:147:HEC:CBC	1.04	2.35	17	2
2:B:40:ARG:CD	1:C:92:ARG:HE	1.04	1.64	19	1
1:C:86:LEU:HD11	3:C:142:HEC:CBD	1.04	1.82	7	2
3:B:147:HEC:CHC	2:D:106:LEU:HD12	1.04	1.77	15	1
2:B:132:LYS:HD3	2:D:146:HIS:O	1.04	1.50	15	1
3:B:147:HEC:C4B	2:D:106:LEU:HD13	1.04	1.83	15	1
2:D:63:HIS:HE1	3:D:147:HEC:CHA	1.03	1.66	19	8
2:B:40:ARG:NH1	1:C:94:ASP:OD1	1.03	1.91	3	1
2:B:106:LEU:HD13	3:B:147:HEC:CHC	1.03	1.83	12	15
2:B:146:HIS:CD2	2:D:135:ALA:O	1.03	2.10	17	1
2:B:63:HIS:HE1	3:B:147:HEC:CHA	1.03	1.66	19	8
2:B:146:HIS:HD2	2:D:139:ASN:CG	1.03	1.56	6	1
1:A:86:LEU:HD11	3:A:142:HEC:CBD	1.03	1.82	7	2
1:A:34:LEU:CD1	2:B:128:ALA:CB	1.03	2.20	18	1
2:D:42:PHE:HB2	3:D:147:HEC:C3A	1.03	1.83	12	1
1:A:96:VAL:CB	2:D:99:ASP:OD2	1.02	2.06	11	2
2:B:106:LEU:HD12	3:B:147:HEC:CHC	1.02	1.81	9	7
2:B:63:HIS:NE2	3:B:147:HEC:C4D	1.02	2.22	16	10
2:D:63:HIS:NE2	3:D:147:HEC:C4D	1.02	2.22	16	9
1:A:48:LEU:HD13	1:A:48:LEU:H	1.02	1.13	11	2
2:B:67:VAL:CG1	3:B:147:HEC:C1B	1.02	2.37	19	2
2:D:67:VAL:CG1	3:D:147:HEC:C1B	1.02	2.37	19	2
1:C:48:LEU:HD13	1:C:48:LEU:H	1.02	1.13	11	2
2:B:106:LEU:HG	3:B:147:HEC:CAB	1.02	1.84	18	1
2:B:99:ASP:HB3	1:C:96:VAL:HG21	1.01	1.26	18	2
1:C:36:PHE:CZ	2:D:131:GLN:NE2	1.01	2.28	13	1
2:D:39:GLN:N	3:D:147:HEC:C1C	1.01	2.23	12	1
1:A:117:PHE:CE1	2:B:116:HIS:CD2	1.01	2.48	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ALA:CB	2:B:122:PHE:CE2	1.01	2.44	8	3
1:A:86:LEU:HD11	3:A:142:HEC:HBD2	1.00	1.13	7	2
1:A:92:ARG:CD	2:D:40:ARG:NE	1.00	2.21	16	2
2:B:42:PHE:HE2	3:B:147:HEC:HMD3	1.00	1.01	2	1
1:A:36:PHE:CZ	2:B:131:GLN:NE2	1.00	2.28	13	1
1:C:117:PHE:CE1	2:D:116:HIS:CD2	1.00	2.48	13	1
2:B:40:ARG:CZ	1:C:92:ARG:HB3	1.00	1.75	17	1
2:B:146:HIS:CD2	2:D:139:ASN:CG	1.00	2.33	6	2
2:B:106:LEU:HD21	3:B:147:HEC:HHC	1.00	1.16	2	1
1:C:34:LEU:HD13	2:D:128:ALA:HB2	1.00	1.34	8	7
2:D:106:LEU:HG	3:D:147:HEC:CAB	1.00	1.84	18	1
1:A:92:ARG:HE	2:D:40:ARG:CD	0.99	1.68	19	1
1:A:41:THR:HG21	2:D:97:HIS:NE2	0.99	1.71	11	2
2:B:40:ARG:HD3	1:C:92:ARG:HE	0.99	1.15	19	1
1:A:101:LEU:HD13	3:A:142:HEC:HHC	0.99	1.28	15	4
2:D:42:PHE:CZ	3:D:147:HEC:HMB2	0.99	1.91	12	1
1:A:101:LEU:HD22	3:A:142:HEC:HBB3	0.99	1.02	15	2
1:C:111:ALA:CB	2:D:122:PHE:CE2	0.99	2.44	8	3
1:A:34:LEU:HD13	2:B:128:ALA:HB2	0.99	1.34	8	7
2:D:38:THR:C	3:D:147:HEC:NC	0.99	2.13	12	1
1:C:32:MET:CE	3:C:142:HEC:CAB	0.98	2.37	12	1
1:C:34:LEU:CD1	2:D:128:ALA:CB	0.98	2.20	18	1
1:C:101:LEU:HD22	3:C:142:HEC:HBB3	0.98	1.02	15	2
2:D:106:LEU:HD13	3:D:147:HEC:CHC	0.98	1.87	6	14
1:C:101:LEU:HD13	3:C:142:HEC:HHC	0.98	1.28	15	4
1:C:31:ARG:NH1	2:D:127:GLN:HG2	0.98	1.72	16	2
2:B:106:LEU:CD2	3:B:147:HEC:CBB	0.98	2.10	19	1
1:A:92:ARG:HB2	2:D:40:ARG:CZ	0.98	1.82	17	2
2:D:106:LEU:CD2	3:D:147:HEC:CBB	0.98	2.10	19	1
1:A:92:ARG:HD3	2:D:40:ARG:HD3	0.97	1.31	18	1
2:B:139:ASN:CG	2:D:146:HIS:HD2	0.97	1.62	6	1
1:A:92:ARG:HD3	2:D:40:ARG:HD2	0.97	1.01	17	2
2:B:42:PHE:HE1	3:B:147:HEC:HBC1	0.97	1.15	12	3
2:D:106:LEU:CD1	3:D:147:HEC:HHC	0.97	1.90	5	11
2:B:40:ARG:HD2	1:C:92:ARG:HD3	0.97	0.99	17	2
1:A:92:ARG:HE	2:D:40:ARG:HD3	0.97	1.20	19	1
1:A:117:PHE:HZ	2:B:116:HIS:NE2	0.96	1.21	13	1
2:B:99:ASP:OD2	1:C:96:VAL:CB	0.96	2.13	11	2
2:B:139:ASN:CG	2:D:146:HIS:CD2	0.96	2.39	6	2
2:D:42:PHE:CB	3:D:147:HEC:CHB	0.96	2.43	12	1
2:B:106:LEU:HD13	3:B:147:HEC:CAB	0.96	1.91	9	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:101:LEU:CD2	3:C:142:HEC:HHC	0.96	1.90	4	3
2:D:106:LEU:HD13	3:D:147:HEC:CAB	0.96	1.91	9	9
2:B:106:LEU:CD1	3:B:147:HEC:HHC	0.95	1.90	5	11
2:D:42:PHE:CE1	3:D:147:HEC:HMB2	0.95	1.95	12	1
1:A:31:ARG:NH1	2:B:127:GLN:HG2	0.95	1.72	16	2
1:A:101:LEU:CD2	3:A:142:HEC:HHC	0.95	1.90	4	3
1:C:40:LYS:O	3:C:142:HEC:C3D	0.95	2.15	12	1
1:A:34:LEU:HB3	2:B:128:ALA:HB2	0.94	1.40	15	5
1:A:41:THR:CG2	2:D:97:HIS:ND1	0.94	2.26	17	1
2:B:3:LEU:HD12	2:B:3:LEU:H	0.94	1.22	6	15
2:B:139:ASN:OD1	2:D:146:HIS:ND1	0.94	2.01	8	1
1:C:34:LEU:HB3	2:D:128:ALA:HB2	0.94	1.39	15	5
2:D:106:LEU:HD13	3:D:147:HEC:C3B	0.94	1.92	9	8
2:B:139:ASN:OD1	2:D:146:HIS:CG	0.94	2.21	8	1
2:B:146:HIS:CG	2:D:139:ASN:OD1	0.94	2.20	8	1
2:B:146:HIS:CD2	2:D:139:ASN:OD1	0.93	2.21	8	2
2:B:63:HIS:CE1	3:B:147:HEC:O1A	0.93	2.21	5	1
1:A:36:PHE:CZ	2:B:131:GLN:OE1	0.93	2.21	2	4
1:C:36:PHE:CZ	2:D:131:GLN:OE1	0.93	2.21	2	4
2:D:42:PHE:CB	3:D:147:HEC:C3A	0.93	2.47	12	1
1:C:31:ARG:HH12	2:D:127:GLN:CG	0.93	1.75	16	1
2:B:42:PHE:HE1	3:B:147:HEC:CBC	0.93	1.75	18	1
1:A:101:LEU:CD2	3:A:142:HEC:CHC	0.93	2.47	4	3
2:B:106:LEU:HD13	3:B:147:HEC:C3B	0.93	1.92	9	9
1:A:111:ALA:CB	2:B:122:PHE:CZ	0.93	2.52	8	1
2:D:3:LEU:HD12	2:D:3:LEU:H	0.93	1.24	4	15
2:B:146:HIS:O	2:D:132:LYS:HG3	0.93	1.62	9	1
2:B:106:LEU:HD11	3:B:147:HEC:HAB	0.92	1.40	2	1
2:D:63:HIS:CE1	3:D:147:HEC:O1A	0.92	2.21	5	1
1:C:111:ALA:CB	2:D:122:PHE:CZ	0.92	2.52	8	1
1:A:101:LEU:CD1	3:A:142:HEC:HHC	0.92	1.94	7	3
1:C:101:LEU:CD1	3:C:142:HEC:HHC	0.92	1.94	7	3
2:B:146:HIS:ND1	2:D:139:ASN:OD1	0.92	2.01	8	1
2:B:132:LYS:HG3	2:D:146:HIS:O	0.92	1.64	9	1
2:D:38:THR:CG2	3:D:147:HEC:HBC1	0.92	1.95	20	1
1:A:38:THR:CG2	2:D:97:HIS:ND1	0.91	2.32	7	1
1:C:46:PHE:CD1	3:C:142:HEC:HMA3	0.91	2.01	12	1
1:C:101:LEU:CD2	3:C:142:HEC:CHC	0.91	2.47	4	3
1:C:40:LYS:O	3:C:142:HEC:C4D	0.91	2.18	12	1
1:A:41:THR:CG2	2:D:97:HIS:NE2	0.91	2.33	11	2
2:B:38:THR:CG2	3:B:147:HEC:HBC1	0.91	1.95	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:97:HIS:NE2	1:C:41:THR:HG21	0.91	1.79	11	2
1:C:36:PHE:HZ	2:D:131:GLN:OE1	0.91	1.47	9	2
1:C:117:PHE:CZ	2:D:116:HIS:CE1	0.90	2.60	4	1
1:A:31:ARG:HH12	2:B:127:GLN:CG	0.90	1.75	16	1
1:A:36:PHE:HZ	2:B:131:GLN:OE1	0.90	1.47	9	2
1:A:92:ARG:HB2	2:D:40:ARG:NE	0.90	1.81	17	1
2:D:42:PHE:HE1	3:D:147:HEC:CBC	0.90	1.75	18	1
2:D:106:LEU:HD11	3:D:147:HEC:HAB	0.90	1.40	2	1
1:A:117:PHE:CZ	2:B:116:HIS:CE1	0.90	2.60	4	1
1:C:101:LEU:HD22	3:C:142:HEC:HBB1	0.89	1.44	15	1
1:A:92:ARG:HD2	2:D:40:ARG:HG2	0.89	1.40	3	2
1:C:36:PHE:HB3	3:C:142:HEC:CMC	0.89	1.96	12	1
2:B:38:THR:HG21	3:B:147:HEC:HBC1	0.89	1.44	20	2
2:B:40:ARG:HD3	1:C:92:ARG:HD3	0.89	1.39	18	1
2:D:42:PHE:CB	3:D:147:HEC:HHB	0.88	1.96	12	1
2:B:106:LEU:HD13	3:B:147:HEC:HHC	0.88	1.44	5	9
2:B:106:LEU:HD13	3:B:147:HEC:C4B	0.88	1.98	9	13
2:B:132:LYS:CD	2:D:146:HIS:O	0.88	2.21	15	1
1:A:92:ARG:NH1	2:D:40:ARG:HB2	0.88	1.82	18	1
1:A:92:ARG:NE	2:D:40:ARG:HG2	0.88	1.84	8	1
2:D:106:LEU:HD13	3:D:147:HEC:C4B	0.88	1.98	9	12
2:B:139:ASN:OD1	2:D:146:HIS:CD2	0.88	2.26	8	2
1:A:65:ALA:HB2	3:A:142:HEC:HMA1	0.88	1.45	9	5
2:B:146:HIS:O	2:D:132:LYS:CD	0.88	2.20	15	1
1:A:92:ARG:CD	2:D:40:ARG:CB	0.88	2.51	19	1
2:B:146:HIS:HE2	2:D:135:ALA:C	0.88	1.71	17	1
3:B:147:HEC:HAB	2:D:106:LEU:HD22	0.88	1.45	15	1
2:B:139:ASN:ND2	2:D:146:HIS:CE1	0.87	2.41	20	1
2:B:40:ARG:NE	1:C:92:ARG:HB2	0.87	1.83	17	1
2:D:106:LEU:HD22	3:D:147:HEC:CAB	0.87	1.98	10	1
2:B:97:HIS:ND1	1:C:38:THR:CG2	0.87	2.37	7	1
1:C:101:LEU:HD12	3:C:142:HEC:HMC3	0.87	1.47	7	1
2:B:106:LEU:HD22	3:B:147:HEC:CAB	0.87	1.98	10	1
2:B:40:ARG:NE	1:C:92:ARG:HD3	0.86	1.83	18	1
1:C:97:ASN:HB3	3:C:142:HEC:HMC1	0.86	1.46	17	1
1:C:65:ALA:HB2	3:C:142:HEC:HMA1	0.86	1.45	9	5
2:B:63:HIS:CE1	3:B:147:HEC:C4D	0.86	2.58	19	7
2:D:63:HIS:CE1	3:D:147:HEC:C4D	0.86	2.58	19	7
2:B:106:LEU:HD12	3:B:147:HEC:HHC	0.86	1.45	9	5
2:B:82:LYS:HZ3	2:D:82:LYS:NZ	0.86	1.65	15	1
1:A:97:ASN:HB3	3:A:142:HEC:HMC1	0.86	1.46	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:117:PHE:HD1	2:D:30:ARG:NH2	0.86	1.69	13	3
2:D:106:LEU:HD13	3:D:147:HEC:HHC	0.86	1.44	5	8
2:B:146:HIS:NE2	2:D:139:ASN:CG	0.86	2.28	8	1
2:B:135:ALA:C	2:D:146:HIS:NE2	0.86	2.28	17	1
2:B:67:VAL:HG22	3:B:147:HEC:C4A	0.85	2.01	9	13
1:A:96:VAL:HG21	2:D:99:ASP:HB2	0.85	1.48	18	1
2:B:3:LEU:N	2:B:3:LEU:HD12	0.85	1.87	17	6
1:C:32:MET:HE2	3:C:142:HEC:HAB	0.85	0.88	12	1
2:D:32:LEU:C	3:D:147:HEC:HMB1	0.85	1.91	15	1
1:A:92:ARG:CD	2:D:40:ARG:HE	0.85	1.80	16	1
2:B:146:HIS:NE2	2:D:139:ASN:OD1	0.85	2.08	8	1
2:D:67:VAL:HG22	3:D:147:HEC:C4A	0.85	2.02	9	12
1:A:117:PHE:HD1	2:B:30:ARG:HH21	0.85	1.14	17	2
2:D:106:LEU:HD12	3:D:147:HEC:HHC	0.85	1.45	9	3
2:B:42:PHE:HE2	3:B:147:HEC:CMD	0.85	1.85	2	1
2:B:63:HIS:HE1	3:B:147:HEC:C1A	0.85	1.84	13	6
2:D:63:HIS:NE2	3:D:147:HEC:CAD	0.85	2.40	19	4
2:D:67:VAL:CG1	3:D:147:HEC:C2B	0.85	2.54	19	3
2:D:42:PHE:HE1	3:D:147:HEC:HBC1	0.85	1.18	17	2
2:D:38:THR:HG21	3:D:147:HEC:HBC1	0.85	1.44	20	2
2:D:42:PHE:HE2	3:D:147:HEC:CMD	0.85	1.85	2	1
1:A:101:LEU:HD12	3:A:142:HEC:HMC3	0.85	1.47	7	1
1:C:36:PHE:O	3:C:142:HEC:CMC	0.85	2.25	12	1
2:B:63:HIS:NE2	3:B:147:HEC:CAD	0.85	2.40	19	4
2:B:40:ARG:HG2	1:C:92:ARG:HD2	0.85	1.46	3	2
1:A:117:PHE:HD1	2:B:30:ARG:NH2	0.84	1.69	17	3
2:B:135:ALA:CB	2:D:146:HIS:O	0.84	2.24	4	1
1:A:92:ARG:NH1	2:D:40:ARG:O	0.84	2.10	17	1
1:A:101:LEU:HD23	3:A:142:HEC:HHC	0.84	1.46	4	1
2:D:3:LEU:N	2:D:3:LEU:HD12	0.84	1.87	17	6
2:B:40:ARG:CB	1:C:92:ARG:CD	0.84	2.55	19	1
1:A:117:PHE:CE1	2:B:116:HIS:HD2	0.84	1.87	13	1
1:A:101:LEU:HD22	3:A:142:HEC:HBB1	0.84	1.44	15	1
2:B:40:ARG:HG2	1:C:92:ARG:NE	0.84	1.88	8	1
2:D:67:VAL:HG22	3:D:147:HEC:NA	0.84	1.88	19	3
2:B:146:HIS:CE1	2:D:139:ASN:ND2	0.84	2.46	20	1
1:C:101:LEU:HD23	3:C:142:HEC:HHC	0.84	1.46	4	1
1:C:117:PHE:CE1	2:D:116:HIS:HD2	0.84	1.87	13	1
2:B:139:ASN:CG	2:D:146:HIS:CE1	0.83	2.52	8	1
2:D:63:HIS:HE1	3:D:147:HEC:C1A	0.83	1.84	13	6
1:A:66:LEU:O	1:A:66:LEU:HD12	0.83	1.73	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:40:LYS:O	3:C:142:HEC:C2D	0.83	2.09	12	1
2:B:67:VAL:HG22	3:B:147:HEC:NA	0.83	1.88	19	4
1:C:39:THR:HB	3:C:142:HEC:CHC	0.83	2.02	12	1
1:C:31:ARG:HH12	2:D:127:GLN:CB	0.83	1.87	16	1
2:B:42:PHE:HZ	3:B:147:HEC:HBC3	0.83	1.28	2	2
1:C:66:LEU:HD12	1:C:66:LEU:O	0.83	1.73	17	2
2:B:146:HIS:NE2	2:D:135:ALA:C	0.83	2.31	17	1
1:A:113:LEU:HD23	1:A:113:LEU:O	0.83	1.74	16	3
1:A:31:ARG:HH12	2:B:127:GLN:CB	0.83	1.87	16	1
2:B:42:PHE:CE1	3:B:147:HEC:HBC3	0.83	2.08	18	2
2:B:139:ASN:CG	2:D:146:HIS:NE2	0.83	2.32	8	1
2:D:42:PHE:CE1	3:D:147:HEC:HBC3	0.83	2.08	18	2
2:D:39:GLN:O	3:D:147:HEC:ND	0.83	2.09	12	1
2:D:42:PHE:CE2	3:D:147:HEC:HMB2	0.83	2.08	12	1
1:A:61:LYS:HB3	3:A:142:HEC:C3A	0.82	2.04	19	9
2:B:63:HIS:CE1	3:B:147:HEC:C1A	0.82	2.62	16	4
2:D:42:PHE:CG	3:D:147:HEC:HHB	0.82	2.08	12	1
2:B:146:HIS:CE1	2:D:139:ASN:CG	0.82	2.51	8	1
2:D:63:HIS:CE1	3:D:147:HEC:C1A	0.82	2.62	16	5
1:A:41:THR:CG2	2:D:97:HIS:CG	0.82	2.61	12	3
1:A:28:ALA:HB1	1:A:104:CYS:SG	0.82	2.14	5	1
1:C:113:LEU:HD23	1:C:113:LEU:O	0.82	1.74	16	3
2:B:66:LYS:HD3	3:B:147:HEC:O2A	0.82	1.74	13	1
2:B:67:VAL:CG1	3:B:147:HEC:C2B	0.82	2.54	19	3
1:C:122:HIS:HB3	2:D:34:VAL:HG13	0.82	1.51	18	3
2:D:106:LEU:HD12	3:D:147:HEC:HAB	0.82	0.82	18	1
1:C:61:LYS:HB3	3:C:142:HEC:C3A	0.82	2.04	19	9
1:A:101:LEU:HD12	3:A:142:HEC:CHC	0.82	2.03	19	2
2:D:66:LYS:HD3	3:D:147:HEC:O2A	0.82	1.74	13	1
2:B:97:HIS:NE2	1:C:41:THR:CG2	0.81	2.42	11	2
1:C:45:HIS:H	3:C:142:HEC:HMA2	0.81	1.04	12	1
2:D:38:THR:H	3:D:147:HEC:HHC	0.81	0.88	12	1
1:C:117:PHE:CE1	2:D:116:HIS:NE2	0.81	2.48	20	1
1:C:48:LEU:CD1	3:C:142:HEC:HHA	0.81	2.04	12	1
1:A:105:LEU:HD12	1:A:105:LEU:O	0.81	1.76	13	3
1:A:129:LEU:O	1:A:129:LEU:HD12	0.81	1.76	7	2
1:C:31:ARG:NH1	2:D:127:GLN:CD	0.81	2.33	16	1
2:D:36:PRO:O	3:D:147:HEC:C2C	0.81	2.29	12	1
1:A:96:VAL:CG2	2:D:99:ASP:OD2	0.81	2.28	11	2
1:C:28:ALA:HB1	1:C:104:CYS:SG	0.81	2.14	5	1
1:A:31:ARG:NH1	2:B:127:GLN:CD	0.81	2.33	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:142:HEC:HBB3	3:C:142:HEC:HMB1	0.81	1.50	11	5
2:D:3:LEU:HD12	2:D:3:LEU:N	0.81	1.91	1	9
1:A:117:PHE:CE1	2:B:116:HIS:NE2	0.81	2.48	20	1
1:C:117:PHE:HD1	2:D:30:ARG:HH21	0.80	1.14	17	2
2:B:40:ARG:HB2	1:C:92:ARG:NH1	0.80	1.90	18	1
2:D:67:VAL:HG13	3:D:147:HEC:CHB	0.80	2.06	19	1
2:B:139:ASN:OD1	2:D:146:HIS:NE2	0.80	2.14	8	1
1:A:122:HIS:HB3	2:B:34:VAL:HG13	0.80	1.51	18	3
1:A:96:VAL:CG2	2:D:99:ASP:CB	0.80	2.57	18	1
1:A:92:ARG:HE	2:D:40:ARG:CB	0.80	1.84	19	2
2:B:146:HIS:O	2:D:135:ALA:CB	0.80	2.30	4	1
1:A:103:HIS:NE2	2:B:35:TYR:OH	0.80	2.14	9	1
2:D:42:PHE:HZ	3:D:147:HEC:HBC3	0.80	1.28	2	2
1:C:129:LEU:O	1:C:129:LEU:HD12	0.80	1.76	7	2
1:C:105:LEU:HD12	1:C:105:LEU:O	0.80	1.76	13	3
1:C:101:LEU:HD12	3:C:142:HEC:CHC	0.80	2.03	19	2
3:A:142:HEC:HBB3	3:A:142:HEC:HMB1	0.80	1.50	11	5
2:D:133:VAL:HG13	2:D:134:VAL:H	0.80	1.37	12	3
1:C:36:PHE:HB3	3:C:142:HEC:HMC3	0.80	1.52	12	1
1:A:118:THR:O	1:A:120:ALA:N	0.80	2.14	10	19
2:D:42:PHE:CE2	3:D:147:HEC:CBC	0.79	2.65	11	1
2:B:67:VAL:HG13	3:B:147:HEC:CHB	0.79	2.06	19	1
1:A:38:THR:HA	2:D:97:HIS:HB3	0.79	1.51	4	1
2:B:135:ALA:HB1	2:D:146:HIS:CG	0.79	2.13	3	1
2:B:135:ALA:O	2:D:146:HIS:NE2	0.79	2.15	17	1
2:B:106:LEU:HG	3:B:147:HEC:C3B	0.79	2.07	18	1
2:B:106:LEU:HD12	3:B:147:HEC:HAB	0.79	0.82	18	1
2:B:3:LEU:HD12	2:B:3:LEU:N	0.79	1.91	1	9
1:A:92:ARG:CD	2:D:40:ARG:HB2	0.79	2.07	19	1
1:A:41:THR:HG23	2:D:97:HIS:CE1	0.79	2.10	17	1
1:A:92:ARG:HH11	2:D:40:ARG:HD2	0.79	1.38	18	1
1:A:111:ALA:HB2	2:B:122:PHE:CZ	0.79	2.10	8	1
1:C:103:HIS:NE2	2:D:35:TYR:OH	0.79	2.15	9	1
2:B:42:PHE:CE2	3:B:147:HEC:CBC	0.79	2.65	11	1
3:B:147:HEC:C2B	2:D:67:VAL:HG13	0.79	2.07	15	1
1:A:31:ARG:HG3	2:B:127:GLN:HE22	0.79	1.38	6	1
1:C:118:THR:O	1:C:120:ALA:N	0.78	2.14	10	19
1:C:31:ARG:HG3	2:D:127:GLN:HE22	0.78	1.38	6	1
2:D:106:LEU:HG	3:D:147:HEC:C3B	0.78	2.07	18	1
1:C:86:LEU:CD1	3:C:142:HEC:CBD	0.78	2.62	7	2
1:A:86:LEU:CD1	3:A:142:HEC:CBD	0.78	2.62	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:139:ASN:HD21	2:D:139:ASN:HD21	0.78	1.19	12	1
2:D:42:PHE:HB3	3:D:147:HEC:HMA1	0.78	0.82	12	1
3:B:147:HEC:C3B	2:D:106:LEU:HD13	0.78	2.07	15	1
2:B:99:ASP:HB2	1:C:96:VAL:HG21	0.78	1.53	18	1
1:C:46:PHE:O	1:C:48:LEU:N	0.78	2.16	19	8
3:B:147:HEC:HH2	2:D:106:LEU:HD13	0.78	1.39	15	1
2:B:133:VAL:HG13	2:B:134:VAL:H	0.78	1.37	12	3
2:D:106:LEU:HD23	3:D:147:HEC:HMC3	0.77	1.54	2	1
2:B:135:ALA:HB3	2:D:146:HIS:O	0.77	1.78	4	1
1:C:111:ALA:HB2	2:D:122:PHE:CZ	0.77	2.10	8	1
1:A:92:ARG:NH2	3:D:147:HEC:CB2	0.77	2.32	12	1
2:D:75:LEU:HD23	2:D:75:LEU:N	0.77	1.94	20	3
1:A:46:PHE:O	1:A:48:LEU:N	0.77	2.16	19	7
2:B:40:ARG:O	1:C:92:ARG:NH1	0.77	2.17	17	1
1:C:101:LEU:HD21	3:C:142:HEC:HBB3	0.77	1.56	2	4
1:C:103:HIS:ND1	2:D:108:ASN:OD1	0.77	2.17	8	2
1:C:36:PHE:CE2	2:D:131:GLN:NE2	0.77	2.50	13	1
1:C:31:ARG:HH21	2:D:127:GLN:HB2	0.77	1.40	15	1
2:B:102:ASN:OD1	3:B:147:HEC:CMC	0.77	2.33	12	1
1:A:65:ALA:CB	3:A:142:HEC:HMA1	0.77	2.10	9	1
2:D:42:PHE:CD1	3:D:147:HEC:HMB2	0.77	2.14	12	1
2:B:106:LEU:HD23	3:B:147:HEC:HMC3	0.77	1.54	2	1
2:B:42:PHE:CZ	3:B:147:HEC:HBC2	0.77	2.13	12	2
2:D:67:VAL:HG22	3:D:147:HEC:NB	0.77	1.95	9	7
1:A:101:LEU:HD21	3:A:142:HEC:HBB3	0.76	1.56	2	4
2:B:82:LYS:NZ	2:D:82:LYS:HZ3	0.76	1.76	15	1
2:B:40:ARG:HD3	1:C:92:ARG:NE	0.76	1.94	19	1
1:A:96:VAL:HG21	2:D:99:ASP:OD2	0.76	1.79	11	2
1:C:65:ALA:CB	3:C:142:HEC:HMA1	0.76	2.10	9	1
1:A:31:ARG:HH21	2:B:127:GLN:HB2	0.76	1.39	15	1
1:A:94:ASP:CG	2:D:40:ARG:NH1	0.76	2.39	3	1
1:A:29:LEU:HD11	1:A:58:HIS:CG	0.76	2.16	4	3
2:B:97:HIS:HB3	1:C:38:THR:HA	0.76	1.55	4	1
1:A:103:HIS:ND1	2:B:108:ASN:OD1	0.76	2.17	8	2
1:C:86:LEU:CD1	3:C:142:HEC:HBD2	0.76	2.06	7	1
2:B:97:HIS:CG	1:C:41:THR:CG2	0.76	2.66	12	3
2:D:42:PHE:HZ	3:D:147:HEC:HBC2	0.76	1.38	17	1
2:B:67:VAL:CG2	3:B:147:HEC:C1B	0.76	2.63	9	3
1:A:65:ALA:HB2	3:A:142:HEC:CMA	0.76	2.11	9	2
2:B:146:HIS:NE2	2:D:135:ALA:O	0.76	2.19	17	1
2:B:146:HIS:CG	2:D:135:ALA:HB1	0.76	2.15	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:75:LEU:HD23	2:B:75:LEU:N	0.76	1.95	4	3
1:C:65:ALA:HB2	3:C:142:HEC:CMA	0.76	2.11	9	1
2:B:42:PHE:HZ	3:B:147:HEC:HBC2	0.75	1.41	12	2
1:A:92:ARG:CD	2:D:40:ARG:HG2	0.75	2.12	8	2
1:C:29:LEU:HD11	1:C:58:HIS:CG	0.75	2.16	4	3
2:B:67:VAL:HG22	3:B:147:HEC:NB	0.75	1.96	9	7
2:B:99:ASP:OD2	1:C:96:VAL:CG2	0.75	2.35	11	2
2:B:106:LEU:CD1	3:B:147:HEC:C4B	0.75	2.64	9	3
1:A:126:ASP:OD1	2:B:35:TYR:CD2	0.75	2.39	13	1
1:A:92:ARG:CD	2:D:40:ARG:HB3	0.75	2.10	19	2
1:A:36:PHE:CE2	2:B:131:GLN:NE2	0.75	2.50	13	1
2:B:146:HIS:O	2:D:135:ALA:HB3	0.75	1.81	4	1
2:D:42:PHE:C	3:D:147:HEC:CMA	0.75	2.52	12	1
2:B:40:ARG:HD2	1:C:92:ARG:HH11	0.75	1.38	18	1
2:B:42:PHE:HE2	3:B:147:HEC:CBC	0.75	1.95	11	1
1:C:61:LYS:HG2	3:C:142:HEC:C2A	0.75	2.12	19	1
1:A:38:THR:O	1:A:41:THR:HG22	0.74	1.83	20	9
2:D:67:VAL:HA	3:D:147:HEC:CHB	0.74	2.12	19	5
2:B:42:PHE:CE2	3:B:147:HEC:HBC3	0.74	2.16	11	1
2:D:42:PHE:HE2	3:D:147:HEC:CBC	0.74	1.95	11	1
2:B:40:ARG:HB3	1:C:92:ARG:CD	0.74	2.12	19	2
1:A:31:ARG:HH11	2:B:127:GLN:HG2	0.74	1.41	10	1
1:C:126:ASP:OD1	2:D:35:TYR:CD2	0.74	2.39	13	1
3:B:147:HEC:C4A	2:D:67:VAL:HG22	0.74	2.12	15	1
1:A:115:ALA:O	1:A:121:VAL:HG21	0.74	1.83	5	9
1:C:31:ARG:HH11	2:D:127:GLN:HG2	0.74	1.41	10	1
2:B:67:VAL:HA	3:B:147:HEC:CHB	0.74	2.12	19	4
1:C:101:LEU:HD22	3:C:142:HEC:CHC	0.74	2.12	18	9
3:C:142:HEC:HMB1	3:C:142:HEC:HBB2	0.74	1.57	16	11
1:C:38:THR:O	1:C:41:THR:HG22	0.74	1.82	20	9
2:B:135:ALA:CB	2:D:146:HIS:HB3	0.74	2.13	3	1
1:C:93:VAL:HG22	1:C:94:ASP:H	0.74	1.42	13	1
3:A:142:HEC:HMB1	3:A:142:HEC:HBB2	0.74	1.57	16	11
2:B:75:LEU:HD23	2:B:75:LEU:H	0.74	1.43	20	3
2:D:38:THR:O	3:D:147:HEC:C1C	0.74	2.35	12	1
2:D:42:PHE:CB	3:D:147:HEC:HMA2	0.74	2.13	12	1
2:D:42:PHE:CE2	3:D:147:HEC:HBC3	0.74	2.16	11	1
1:C:115:ALA:O	1:C:121:VAL:HG21	0.73	1.83	5	9
2:D:39:GLN:O	3:D:147:HEC:C1D	0.73	2.36	12	1
1:C:101:LEU:HD22	3:C:142:HEC:HHC	0.73	1.60	18	4
1:A:101:LEU:HD22	3:A:142:HEC:CHC	0.73	2.12	18	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:132:LYS:HG2	2:D:146:HIS:OXT	0.73	1.84	3	1
2:D:75:LEU:HD23	2:D:75:LEU:H	0.73	1.43	20	3
2:B:146:HIS:CD2	2:D:2:HIS:CD2	0.73	2.74	15	1
2:B:99:ASP:OD2	1:C:96:VAL:HG21	0.73	1.83	11	2
1:A:61:LYS:HG2	3:A:142:HEC:C2A	0.73	2.12	19	1
1:A:101:LEU:HD22	3:A:142:HEC:HHC	0.73	1.60	18	4
2:D:67:VAL:CG2	3:D:147:HEC:C1B	0.73	2.63	9	3
2:B:139:ASN:OD1	2:D:146:HIS:O	0.73	2.06	6	1
1:A:93:VAL:HG22	1:A:94:ASP:H	0.73	1.41	13	1
2:B:146:HIS:HD2	2:D:2:HIS:CE1	0.73	1.97	15	1
2:B:106:LEU:CG	3:B:147:HEC:HBB3	0.73	2.13	19	1
2:D:106:LEU:CG	3:D:147:HEC:HBB3	0.73	2.13	19	1
1:A:13:ALA:O	1:A:17:VAL:HG23	0.73	1.84	2	17
2:B:40:ARG:HD2	1:C:92:ARG:NH1	0.73	1.98	18	1
1:C:103:HIS:CG	2:D:108:ASN:HD21	0.73	2.01	20	1
2:B:146:HIS:O	2:D:132:LYS:CG	0.72	2.36	9	2
2:D:57:ASN:N	2:D:58:PRO:CD	0.72	2.52	19	1
1:C:36:PHE:O	3:C:142:HEC:HMC1	0.72	1.83	12	1
2:B:40:ARG:NH1	1:C:94:ASP:CG	0.72	2.43	3	1
2:D:42:PHE:CG	3:D:147:HEC:CHB	0.72	2.70	12	1
2:B:42:PHE:HE2	3:B:147:HEC:HBC1	0.72	1.44	11	1
2:D:63:HIS:HE1	3:D:147:HEC:C4D	0.72	1.94	19	1
1:A:103:HIS:CG	2:B:108:ASN:HD21	0.72	2.01	20	1
3:B:147:HEC:C1C	2:D:106:LEU:HD12	0.72	2.14	15	1
2:B:133:VAL:HG13	2:B:134:VAL:N	0.72	1.99	9	4
2:D:106:LEU:CB	3:D:147:HEC:CAB	0.72	2.67	18	1
2:D:106:LEU:HD21	3:D:147:HEC:C4B	0.72	2.15	2	1
1:A:31:ARG:CG	2:B:127:GLN:HE22	0.72	1.97	6	1
1:A:121:VAL:HG13	1:A:122:HIS:N	0.72	2.00	17	18
1:A:86:LEU:HD21	3:A:142:HEC:HBD2	0.72	1.59	12	2
1:C:39:THR:CB	3:C:142:HEC:CHC	0.72	2.60	12	1
2:D:42:PHE:CE1	3:D:147:HEC:CMB	0.72	2.72	12	1
2:B:106:LEU:CB	3:B:147:HEC:CAB	0.72	2.67	18	1
1:A:84:SER:O	1:A:88:ALA:HB3	0.71	1.84	4	4
2:B:135:ALA:CB	2:D:146:HIS:NE2	0.71	2.52	17	1
1:A:92:ARG:NH1	2:D:40:ARG:HD2	0.71	1.98	18	1
2:D:106:LEU:HD23	3:D:147:HEC:HHC	0.71	1.60	2	1
1:C:31:ARG:CG	2:D:127:GLN:HE22	0.71	1.97	6	1
1:C:84:SER:O	1:C:88:ALA:HB3	0.71	1.84	4	4
1:A:113:LEU:HD12	1:A:114:PRO:O	0.71	1.85	18	2
2:B:146:HIS:O	2:D:139:ASN:OD1	0.71	2.07	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:45:HIS:H	3:C:142:HEC:CMA	0.71	1.89	12	1
1:C:76:MET:N	1:C:77:PRO:CD	0.71	2.54	5	20
2:B:14:LEU:O	2:B:18:VAL:HG23	0.71	1.85	8	5
1:A:48:LEU:H	1:A:48:LEU:CD1	0.71	1.93	9	5
1:A:96:VAL:HG11	2:D:99:ASP:HB3	0.71	1.62	9	1
2:D:14:LEU:O	2:D:18:VAL:HG23	0.71	1.85	8	5
1:C:35:SER:OG	2:D:131:GLN:OE1	0.71	2.09	16	1
1:A:38:THR:HB	2:D:97:HIS:HB3	0.71	1.61	19	1
2:B:106:LEU:HD21	3:B:147:HEC:C4B	0.71	2.15	2	1
1:C:13:ALA:O	1:C:17:VAL:HG23	0.71	1.84	2	17
2:B:2:HIS:CE1	2:D:146:HIS:HD2	0.71	2.01	15	1
3:B:147:HEC:C1B	2:D:67:VAL:HG13	0.71	2.15	15	1
2:B:57:ASN:N	2:B:58:PRO:CD	0.71	2.52	19	1
2:D:63:HIS:CE1	3:D:147:HEC:CGA	0.71	2.74	5	1
2:D:42:PHE:HE2	3:D:147:HEC:HBC1	0.71	1.44	11	1
1:A:126:ASP:OD1	2:B:35:TYR:CE2	0.71	2.44	13	1
1:C:113:LEU:HD12	1:C:114:PRO:O	0.71	1.85	18	2
2:D:133:VAL:HG13	2:D:134:VAL:N	0.71	1.99	9	4
2:B:97:HIS:CE1	1:C:41:THR:HG23	0.71	2.18	17	1
2:B:135:ALA:CB	2:D:146:HIS:CE1	0.71	2.73	17	1
2:B:135:ALA:HB1	2:D:146:HIS:CE1	0.71	2.21	17	1
1:C:121:VAL:HG13	1:C:122:HIS:N	0.71	2.00	13	18
2:B:2:HIS:CD2	2:D:146:HIS:CD2	0.71	2.77	15	1
1:A:106:LEU:HD12	1:A:122:HIS:CE1	0.70	2.21	4	1
2:D:42:PHE:CZ	3:D:147:HEC:CMB	0.70	2.73	12	1
2:B:40:ARG:HB2	1:C:92:ARG:CD	0.70	2.13	19	1
1:A:76:MET:N	1:A:77:PRO:CD	0.70	2.54	5	20
1:A:35:SER:OG	2:B:131:GLN:OE1	0.70	2.09	16	1
1:C:86:LEU:C	1:C:86:LEU:HD13	0.70	2.07	7	2
1:C:126:ASP:OD1	2:D:35:TYR:CE2	0.70	2.44	13	1
2:B:63:HIS:CE1	3:B:147:HEC:CGA	0.70	2.74	5	1
1:A:92:ARG:HE	2:D:40:ARG:CG	0.70	1.99	19	2
1:A:92:ARG:NE	2:D:40:ARG:HD3	0.70	1.99	19	1
1:A:92:ARG:CB	2:D:40:ARG:NE	0.70	2.55	18	2
1:A:86:LEU:C	1:A:86:LEU:HD13	0.70	2.07	7	2
1:A:38:THR:CB	2:D:97:HIS:HB3	0.70	2.17	19	2
2:B:106:LEU:CD2	3:B:147:HEC:HAB	0.69	2.17	3	6
2:D:32:LEU:HB3	3:D:147:HEC:HMB2	0.69	1.62	15	1
2:B:132:LYS:CG	2:D:146:HIS:O	0.69	2.38	9	2
2:D:38:THR:O	3:D:147:HEC:NC	0.69	2.19	12	1
1:A:101:LEU:CD2	3:A:142:HEC:HBB2	0.69	2.16	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:34:LEU:HD12	2:D:128:ALA:HB2	0.69	1.65	7	2
1:C:36:PHE:CE1	2:D:131:GLN:OE1	0.69	2.46	13	1
2:B:106:LEU:HD23	3:B:147:HEC:HHC	0.69	1.60	2	1
1:C:106:LEU:HD12	1:C:122:HIS:CE1	0.69	2.21	4	1
1:C:36:PHE:O	3:C:142:HEC:C2C	0.69	2.29	12	1
2:B:106:LEU:C	2:B:106:LEU:HD13	0.69	2.08	18	1
2:D:67:VAL:CG2	3:D:147:HEC:CHB	0.69	2.68	9	2
1:C:46:PHE:CE1	3:C:142:HEC:HMA3	0.69	2.22	12	1
2:D:63:HIS:NE2	3:D:147:HEC:C1A	0.69	2.55	16	1
2:B:139:ASN:HD21	2:D:139:ASN:ND2	0.69	1.84	3	2
1:A:36:PHE:CE1	2:B:131:GLN:OE1	0.69	2.46	13	1
1:C:117:PHE:HE1	2:D:116:HIS:HE2	0.69	1.29	20	1
1:A:6:ASP:O	1:A:10:VAL:HG23	0.68	1.89	6	5
1:C:97:ASN:HB3	3:C:142:HEC:CMC	0.68	2.19	17	1
2:D:106:LEU:C	2:D:106:LEU:HD13	0.68	2.08	18	1
2:B:99:ASP:CB	1:C:96:VAL:CG2	0.68	2.63	18	1
2:B:68:LEU:O	2:B:68:LEU:HD23	0.68	1.89	20	7
2:B:146:HIS:OXT	2:D:132:LYS:HG2	0.68	1.88	3	1
1:A:92:ARG:HE	2:D:40:ARG:HG2	0.68	1.49	8	1
2:D:106:LEU:CD1	3:D:147:HEC:C4B	0.68	2.64	9	3
1:C:85:ASP:O	1:C:89:HIS:N	0.68	2.27	11	6
2:B:63:HIS:NE2	3:B:147:HEC:C1A	0.68	2.55	16	1
2:B:96:LEU:O	2:B:97:HIS:ND1	0.68	2.27	14	6
1:C:48:LEU:H	1:C:48:LEU:HD23	0.68	1.49	3	2
1:C:61:LYS:HG2	3:C:142:HEC:CAA	0.68	2.19	19	3
1:C:48:LEU:HD13	1:C:48:LEU:N	0.68	1.97	11	2
1:C:119:PRO:HA	2:D:33:VAL:HG13	0.68	1.64	13	3
1:C:115:ALA:O	1:C:116:GLU:CB	0.68	2.42	1	17
1:C:6:ASP:O	1:C:10:VAL:HG23	0.68	1.89	6	5
1:A:31:ARG:HG3	2:B:127:GLN:NE2	0.68	2.03	6	1
1:C:93:VAL:HG12	1:C:94:ASP:N	0.68	2.04	18	3
1:A:119:PRO:HA	2:B:33:VAL:HG13	0.68	1.64	13	3
2:B:40:ARG:HG2	1:C:92:ARG:CD	0.68	2.19	8	2
1:A:92:ARG:HH22	3:D:147:HEC:HBD2	0.68	0.63	12	1
1:A:101:LEU:CD1	3:A:142:HEC:HBB3	0.68	2.19	15	1
1:A:97:ASN:HB3	3:A:142:HEC:CMC	0.68	2.19	17	1
1:A:61:LYS:HG2	3:A:142:HEC:CAA	0.67	2.19	19	3
1:A:61:LYS:CG	3:A:142:HEC:C2A	0.67	2.71	19	1
1:C:31:ARG:HG3	2:D:127:GLN:NE2	0.67	2.03	6	1
1:A:111:ALA:HB1	2:B:122:PHE:CZ	0.67	2.23	8	1
2:B:40:ARG:CG	1:C:92:ARG:HE	0.67	2.02	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:101:LEU:CD2	3:C:142:HEC:HBB2	0.67	2.16	15	1
1:C:61:LYS:CG	3:C:142:HEC:C2A	0.67	2.71	19	1
2:B:38:THR:HG21	3:B:147:HEC:CBC	0.67	2.19	20	1
2:B:139:ASN:ND2	2:D:139:ASN:HD21	0.67	1.87	3	2
1:A:34:LEU:HD12	2:B:128:ALA:HB2	0.67	1.64	7	2
1:C:101:LEU:CD1	3:C:142:HEC:HBB3	0.67	2.20	15	1
1:A:115:ALA:O	1:A:116:GLU:CB	0.67	2.43	5	17
1:A:94:ASP:HB2	2:D:99:ASP:OD2	0.67	1.89	5	1
3:B:147:HEC:CHA	2:D:63:HIS:CE1	0.67	2.78	15	1
1:A:38:THR:CG2	2:D:97:HIS:HB3	0.67	2.19	19	1
2:D:38:THR:CA	3:D:147:HEC:C1C	0.67	2.48	12	1
2:B:82:LYS:HZ3	2:D:82:LYS:HZ3	0.67	1.25	15	1
2:D:38:THR:HG21	3:D:147:HEC:CBC	0.67	2.19	20	1
1:A:38:THR:CA	2:D:97:HIS:HB3	0.67	2.19	4	1
1:C:103:HIS:ND1	2:D:108:ASN:ND2	0.67	2.43	20	2
1:A:92:ARG:HD2	2:D:40:ARG:HB3	0.67	1.66	19	2
2:B:146:HIS:NE2	2:D:135:ALA:CB	0.67	2.57	17	1
1:A:85:ASP:O	1:A:89:HIS:N	0.67	2.27	11	6
2:D:96:LEU:O	2:D:97:HIS:ND1	0.67	2.27	14	7
2:D:106:LEU:CD2	3:D:147:HEC:HAB	0.67	2.19	5	5
2:D:67:VAL:HG13	3:D:147:HEC:CMB	0.66	2.20	9	3
1:A:93:VAL:HG12	1:A:94:ASP:N	0.66	2.04	18	3
1:A:48:LEU:HD13	1:A:48:LEU:N	0.66	1.97	11	2
1:A:103:HIS:ND1	2:B:108:ASN:ND2	0.66	2.43	20	2
1:A:92:ARG:HD3	2:D:40:ARG:HE	0.66	0.88	16	1
2:D:68:LEU:O	2:D:68:LEU:HD23	0.66	1.89	20	7
2:B:146:HIS:HB3	2:D:135:ALA:CB	0.66	2.18	3	1
1:C:34:LEU:HD12	2:D:128:ALA:CA	0.66	2.19	18	1
2:D:116:HIS:ND1	2:D:116:HIS:N	0.66	2.43	9	1
2:B:106:LEU:HB3	3:B:147:HEC:HAB	0.66	1.66	13	2
2:B:40:ARG:NE	1:C:92:ARG:CD	0.66	2.52	18	1
1:C:119:PRO:HA	2:D:33:VAL:CG1	0.66	2.20	17	2
1:C:61:LYS:CG	3:C:142:HEC:CAA	0.66	2.74	19	2
1:A:48:LEU:H	1:A:48:LEU:HD23	0.66	1.49	3	2
1:C:31:ARG:HH11	2:D:127:GLN:CD	0.66	1.94	16	1
1:A:93:VAL:HG22	1:A:94:ASP:N	0.66	2.05	13	3
1:A:31:ARG:HH11	2:B:127:GLN:CD	0.66	1.94	16	1
1:C:48:LEU:H	1:C:48:LEU:CD1	0.66	1.93	9	5
1:A:119:PRO:HA	2:B:33:VAL:CG1	0.66	2.20	17	3
1:A:122:HIS:CD2	2:B:112:CYS:SG	0.66	2.89	17	1
1:A:92:ARG:HD2	2:D:40:ARG:HD2	0.66	1.62	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:34:LEU:CD1	2:D:128:ALA:CA	0.66	2.74	18	1
1:C:93:VAL:HG22	1:C:94:ASP:N	0.66	2.05	13	3
2:D:38:THR:O	3:D:147:HEC:C4C	0.66	2.44	12	1
2:B:106:LEU:HD23	3:B:147:HEC:CMC	0.66	2.21	2	1
1:A:104:CYS:SG	1:A:105:LEU:N	0.66	2.68	5	1
1:C:104:CYS:SG	1:C:105:LEU:N	0.66	2.68	5	1
2:B:146:HIS:CE1	2:D:135:ALA:CB	0.66	2.79	17	1
1:A:34:LEU:C	1:A:34:LEU:HD12	0.65	2.11	9	2
1:C:101:LEU:CB	3:C:142:HEC:HMC3	0.65	2.21	2	1
2:B:40:ARG:HG2	1:C:92:ARG:HE	0.65	1.50	8	1
2:B:48:LEU:N	2:B:48:LEU:HD12	0.65	2.07	16	5
2:D:106:LEU:HB3	3:D:147:HEC:HAB	0.65	1.66	13	2
1:C:111:ALA:HB1	2:D:122:PHE:CZ	0.65	2.23	8	1
1:C:105:LEU:HD12	1:C:105:LEU:C	0.65	2.12	16	2
1:C:34:LEU:HD12	1:C:34:LEU:C	0.65	2.11	9	3
2:D:33:VAL:HG13	2:D:34:VAL:N	0.65	2.06	3	2
1:A:61:LYS:CG	3:A:142:HEC:CAA	0.65	2.74	19	2
1:A:34:LEU:CD1	2:B:128:ALA:CA	0.65	2.74	18	1
1:A:101:LEU:CB	3:A:142:HEC:HMC3	0.65	2.21	2	1
2:B:116:HIS:ND1	2:B:116:HIS:N	0.65	2.43	9	1
1:A:105:LEU:C	1:A:105:LEU:HD12	0.65	2.12	16	1
1:A:115:ALA:O	1:A:116:GLU:CG	0.65	2.45	6	11
1:C:45:HIS:CG	1:C:45:HIS:O	0.65	2.50	1	8
2:B:146:HIS:CG	2:D:2:HIS:NE2	0.65	2.56	15	1
1:C:122:HIS:CD2	2:D:112:CYS:SG	0.65	2.89	17	1
2:B:63:HIS:HE1	3:B:147:HEC:C4D	0.65	1.94	19	1
2:B:33:VAL:HG13	2:B:34:VAL:N	0.65	2.06	3	2
2:B:67:VAL:HG13	3:B:147:HEC:CMB	0.65	2.20	9	4
1:C:36:PHE:HD2	3:C:142:HEC:CMC	0.65	2.04	12	1
3:B:147:HEC:CAB	2:D:106:LEU:HD13	0.65	2.22	15	1
2:B:135:ALA:CB	2:D:146:HIS:OXT	0.65	2.44	18	1
1:A:117:PHE:HE1	2:B:30:ARG:NH2	0.65	1.88	3	1
1:A:83:LEU:HD12	1:A:83:LEU:C	0.65	2.12	7	1
2:B:130:TYR:CG	2:B:131:GLN:N	0.65	2.65	9	1
2:D:81:LEU:HD23	2:D:81:LEU:N	0.65	2.07	10	1
1:A:129:LEU:HD12	1:A:129:LEU:C	0.65	2.12	20	2
1:C:83:LEU:C	1:C:83:LEU:HD12	0.65	2.12	7	1
1:A:31:ARG:NH1	2:B:127:GLN:OE1	0.65	2.30	10	1
2:B:81:LEU:HD23	2:B:81:LEU:N	0.65	2.07	10	1
1:C:31:ARG:NH1	2:D:127:GLN:OE1	0.65	2.30	10	1
1:A:45:HIS:CG	1:A:45:HIS:O	0.65	2.50	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:63:HIS:CE1	3:B:147:HEC:HHA	0.65	2.26	12	4
2:B:66:LYS:HD3	3:B:147:HEC:CGA	0.65	2.22	14	1
2:B:63:HIS:NE2	3:B:147:HEC:C3D	0.64	2.60	13	9
2:D:106:LEU:HD23	3:D:147:HEC:CMC	0.64	2.21	2	1
1:C:129:LEU:HD12	1:C:129:LEU:C	0.64	2.12	20	2
2:D:48:LEU:HD12	2:D:48:LEU:N	0.64	2.07	16	5
2:D:130:TYR:CG	2:D:131:GLN:N	0.64	2.65	9	1
2:B:102:ASN:OD1	3:B:147:HEC:HMC2	0.64	1.91	12	1
2:D:66:LYS:HD3	3:D:147:HEC:CGA	0.64	2.22	14	1
1:A:117:PHE:HE1	2:B:116:HIS:NE2	0.64	1.89	20	1
2:D:63:HIS:NE2	3:D:147:HEC:C3D	0.64	2.60	13	8
1:A:137:THR:HG22	1:A:137:THR:O	0.64	1.91	12	1
2:D:42:PHE:CD2	3:D:147:HEC:HMB2	0.64	2.27	12	1
1:A:24:TYR:CD1	1:A:112:HIS:CD2	0.64	2.86	7	3
1:C:137:THR:HG22	1:C:137:THR:O	0.64	1.91	12	1
2:B:3:LEU:HD23	2:B:132:LYS:NZ	0.64	2.08	15	1
2:B:97:HIS:CG	2:B:97:HIS:O	0.64	2.51	16	4
2:B:63:HIS:HE1	3:B:147:HEC:HAA1	0.64	1.52	16	1
2:B:93:CYS:SG	2:B:94:ASP:N	0.64	2.70	10	2
1:A:24:TYR:CZ	1:A:112:HIS:CE1	0.64	2.85	16	1
1:C:115:ALA:O	1:C:116:GLU:CG	0.64	2.45	6	11
1:C:24:TYR:CD1	1:C:112:HIS:CD2	0.64	2.86	7	3
2:D:93:CYS:SG	2:D:94:ASP:N	0.64	2.70	10	2
2:D:97:HIS:CG	2:D:97:HIS:O	0.64	2.51	16	4
2:D:3:LEU:HD23	2:D:132:LYS:NZ	0.64	2.08	15	1
2:B:146:HIS:CE1	2:D:135:ALA:HB1	0.64	2.27	17	1
1:A:96:VAL:CG2	2:D:99:ASP:HB2	0.64	2.21	18	1
2:B:3:LEU:N	2:B:3:LEU:CD1	0.64	2.59	1	13
1:A:109:LEU:HD12	1:A:109:LEU:C	0.64	2.14	16	1
1:C:24:TYR:CZ	1:C:112:HIS:CE1	0.64	2.85	16	1
2:B:101:GLU:OE2	2:D:101:GLU:OE2	0.63	2.15	6	1
1:A:101:LEU:HD12	3:A:142:HEC:CMC	0.63	2.22	7	1
2:B:99:ASP:HB3	1:C:96:VAL:HG11	0.63	1.68	9	1
1:A:109:LEU:HD12	1:A:109:LEU:O	0.63	1.93	16	1
1:A:34:LEU:HD12	2:B:128:ALA:CA	0.63	2.19	18	1
3:B:147:HEC:HMD3	2:D:42:PHE:CE2	0.63	2.28	15	1
1:C:109:LEU:HD12	1:C:109:LEU:O	0.63	1.93	16	1
2:B:40:ARG:CG	1:C:92:ARG:NE	0.63	2.62	19	1
1:A:121:VAL:HG13	1:A:122:HIS:H	0.63	1.53	17	3
1:A:129:LEU:CD2	3:A:142:HEC:HBB1	0.63	2.24	13	2
2:B:146:HIS:HB2	2:D:139:ASN:HD21	0.63	1.51	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:38:THR:CG2	3:B:147:HEC:CBC	0.63	2.74	20	1
1:A:69:ALA:O	1:A:73:VAL:N	0.63	2.31	17	17
1:C:109:LEU:HD12	1:C:109:LEU:C	0.63	2.13	16	1
2:D:63:HIS:HE1	3:D:147:HEC:HAA1	0.63	1.52	16	1
2:B:97:HIS:HB3	1:C:38:THR:HB	0.63	1.69	19	1
1:C:101:LEU:HD12	3:C:142:HEC:CMC	0.63	2.22	7	1
3:B:147:HEC:CHB	2:D:67:VAL:HG22	0.63	2.23	15	1
2:B:135:ALA:O	2:D:146:HIS:HD2	0.63	1.71	17	1
2:B:135:ALA:HB1	2:D:146:HIS:CB	0.63	2.24	3	1
2:B:139:ASN:HD22	2:D:146:HIS:CE1	0.63	2.08	20	1
2:D:38:THR:CG2	3:D:147:HEC:CBC	0.63	2.74	20	1
1:C:129:LEU:CD2	3:C:142:HEC:HBB1	0.63	2.24	16	2
2:B:40:ARG:NE	1:C:92:ARG:CB	0.63	2.61	18	2
1:C:129:LEU:O	1:C:133:SER:N	0.63	2.31	18	14
1:A:113:LEU:HD12	1:A:113:LEU:O	0.63	1.94	2	3
2:D:67:VAL:CG2	3:D:147:HEC:C4A	0.63	2.77	9	2
2:B:146:HIS:CE1	2:D:139:ASN:HD22	0.63	2.10	20	1
2:B:42:PHE:CD2	2:B:45:PHE:CE1	0.62	2.88	15	2
1:A:3:SER:N	1:A:4:PRO:CD	0.62	2.62	10	11
1:A:101:LEU:CD2	3:A:142:HEC:HAB	0.62	2.24	11	2
1:A:36:PHE:CZ	2:B:131:GLN:CD	0.62	2.73	13	1
1:A:92:ARG:NH2	2:D:40:ARG:CD	0.62	2.62	15	1
1:A:129:LEU:O	1:A:133:SER:N	0.62	2.31	18	14
2:B:33:VAL:HG13	2:B:34:VAL:H	0.62	1.54	3	1
1:C:24:TYR:CE1	1:C:112:HIS:CD2	0.62	2.88	6	3
1:C:101:LEU:CD2	3:C:142:HEC:HAB	0.62	2.24	11	2
1:C:36:PHE:CZ	2:D:131:GLN:CD	0.62	2.73	13	1
2:B:40:ARG:HB3	1:C:92:ARG:HD2	0.62	1.70	19	2
2:B:139:ASN:HD21	2:D:146:HIS:HB2	0.62	1.53	17	1
2:B:97:HIS:HB3	1:C:38:THR:CG2	0.62	2.23	19	1
1:A:46:PHE:O	1:A:47:ASP:C	0.62	2.37	17	11
1:C:83:LEU:HD12	1:C:83:LEU:O	0.62	1.95	7	1
2:B:67:VAL:CG2	3:B:147:HEC:C4A	0.62	2.77	9	3
1:C:36:PHE:CD2	3:C:142:HEC:CMC	0.62	2.82	12	1
1:C:69:ALA:O	1:C:73:VAL:N	0.62	2.31	17	16
1:C:72:HIS:O	1:C:74:ASP:N	0.62	2.33	15	20
2:D:106:LEU:C	2:D:106:LEU:HD23	0.62	2.15	3	3
1:C:103:HIS:CB	2:D:108:ASN:HD21	0.62	2.08	10	2
2:D:42:PHE:CG	3:D:147:HEC:HMB2	0.62	2.29	12	1
2:B:146:HIS:OXT	2:D:135:ALA:CB	0.62	2.48	18	1
1:C:103:HIS:CG	2:D:108:ASN:ND2	0.62	2.67	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:TYR:CD1	1:A:112:HIS:NE2	0.62	2.68	7	2
1:C:3:SER:N	1:C:4:PRO:CD	0.62	2.62	10	10
1:C:45:HIS:ND1	1:C:45:HIS:C	0.62	2.53	1	8
1:A:86:LEU:CD1	3:A:142:HEC:HBD2	0.62	2.06	7	1
1:C:39:THR:N	3:C:142:HEC:CAC	0.62	2.63	12	1
1:C:31:ARG:HH22	2:D:124:PRO:HA	0.62	1.55	15	1
2:B:40:ARG:NH2	1:C:92:ARG:CB	0.62	2.63	17	1
1:A:103:HIS:CG	2:B:108:ASN:ND2	0.62	2.67	20	1
1:A:24:TYR:CE1	1:A:112:HIS:CD2	0.62	2.88	6	3
1:C:46:PHE:CE1	3:C:142:HEC:CMA	0.62	2.83	12	1
1:A:72:HIS:O	1:A:74:ASP:N	0.62	2.33	1	20
2:B:67:VAL:CG2	3:B:147:HEC:CHB	0.62	2.68	9	2
2:B:31:LEU:CD2	3:B:147:HEC:HBC2	0.62	2.25	10	1
1:C:36:PHE:HB3	3:C:142:HEC:HMC1	0.62	1.72	12	1
1:A:101:LEU:CG	3:A:142:HEC:HBB3	0.62	2.24	15	1
2:D:33:VAL:HG13	2:D:34:VAL:H	0.61	1.54	3	1
2:D:96:LEU:O	2:D:97:HIS:CD2	0.61	2.53	5	4
1:A:101:LEU:HD23	3:A:142:HEC:HAB	0.61	1.71	8	2
2:D:117:HIS:ND1	2:D:118:PHE:CZ	0.61	2.69	10	1
2:D:63:HIS:CE1	3:D:147:HEC:HHA	0.61	2.26	18	3
1:C:93:VAL:HG12	1:C:94:ASP:H	0.61	1.53	18	1
2:B:106:LEU:HD23	2:B:106:LEU:C	0.61	2.15	3	3
2:B:97:HIS:HB3	1:C:38:THR:CB	0.61	2.24	19	2
2:B:96:LEU:O	2:B:97:HIS:CD2	0.61	2.53	5	4
1:A:83:LEU:HD12	1:A:83:LEU:O	0.61	1.95	7	1
2:B:117:HIS:ND1	2:B:118:PHE:CZ	0.61	2.68	10	1
1:A:115:ALA:O	1:A:116:GLU:HB2	0.61	1.95	7	15
1:C:34:LEU:HD12	1:C:35:SER:N	0.61	2.10	1	4
1:C:118:THR:C	1:C:120:ALA:H	0.61	1.99	18	19
2:B:96:LEU:C	2:B:97:HIS:CG	0.61	2.73	17	6
2:D:42:PHE:CD2	2:D:45:PHE:CE1	0.61	2.88	15	2
1:C:24:TYR:CD1	1:C:112:HIS:NE2	0.61	2.68	7	2
3:B:147:HEC:C4B	2:D:106:LEU:CD1	0.61	2.60	15	1
1:A:93:VAL:HG12	1:A:94:ASP:H	0.61	1.53	18	1
1:C:113:LEU:HD12	1:C:113:LEU:O	0.61	1.94	2	3
2:B:135:ALA:HB1	2:D:146:HIS:HB3	0.61	1.71	3	1
1:C:50:HIS:ND1	1:C:51:GLY:N	0.61	2.48	11	4
1:C:39:THR:N	3:C:142:HEC:C3C	0.61	2.64	12	1
2:D:42:PHE:CA	3:D:147:HEC:HMA2	0.61	2.24	12	1
1:C:101:LEU:CG	3:C:142:HEC:HBB3	0.61	2.24	15	1
1:C:112:HIS:CG	1:C:113:LEU:N	0.61	2.68	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:135:ALA:HB1	2:D:146:HIS:NE2	0.61	2.10	17	1
2:D:31:LEU:CD2	3:D:147:HEC:HBC2	0.61	2.25	10	1
1:A:31:ARG:HH22	2:B:124:PRO:HA	0.61	1.55	15	1
2:B:97:HIS:HB3	1:C:38:THR:CA	0.61	2.25	4	1
2:D:42:PHE:CE1	3:D:147:HEC:HMD3	0.61	2.31	4	2
1:C:46:PHE:O	1:C:47:ASP:C	0.61	2.37	17	10
1:A:69:ALA:HB1	1:A:76:MET:SD	0.61	2.36	18	9
2:D:96:LEU:O	2:D:97:HIS:CG	0.61	2.54	20	11
1:A:52:SER:O	1:A:53:ALA:HB3	0.61	1.96	3	13
2:B:91:LEU:HD23	2:B:91:LEU:C	0.61	2.16	12	2
1:C:39:THR:H	3:C:142:HEC:CAC	0.61	2.08	12	1
1:C:121:VAL:HG13	1:C:122:HIS:H	0.61	1.53	17	3
3:B:147:HEC:NA	2:D:67:VAL:HG22	0.61	2.10	15	1
2:B:67:VAL:HG13	3:B:147:HEC:NB	0.61	2.05	19	1
1:A:118:THR:C	1:A:120:ALA:H	0.61	1.99	10	19
1:A:101:LEU:HB2	3:A:142:HEC:HMC3	0.61	1.73	2	2
2:B:96:LEU:O	2:B:97:HIS:CG	0.61	2.54	6	11
1:C:120:ALA:O	1:C:124:SER:N	0.61	2.33	2	16
2:B:99:ASP:OD2	1:C:94:ASP:HB2	0.61	1.96	5	1
1:C:100:LEU:HD12	1:C:100:LEU:N	0.61	2.11	3	3
2:B:3:LEU:HD13	2:B:8:LYS:HB3	0.61	1.73	6	6
2:D:96:LEU:C	2:D:97:HIS:CG	0.61	2.73	17	6
1:C:101:LEU:HD23	3:C:142:HEC:HAB	0.61	1.71	8	2
1:A:103:HIS:CB	2:B:108:ASN:HD21	0.61	2.08	10	2
2:D:91:LEU:C	2:D:91:LEU:HD23	0.61	2.16	12	2
1:A:100:LEU:HD12	1:A:100:LEU:N	0.61	2.11	3	2
1:A:41:THR:CB	2:D:97:HIS:CE1	0.61	2.83	12	1
1:A:112:HIS:CG	1:A:113:LEU:H	0.61	2.14	16	1
1:C:34:LEU:HD11	2:D:128:ALA:N	0.61	2.11	18	1
1:C:24:TYR:CE1	1:C:112:HIS:CG	0.61	2.88	20	1
1:A:72:HIS:O	1:A:73:VAL:HG12	0.60	1.95	13	20
1:C:115:ALA:O	1:C:116:GLU:HB2	0.60	1.95	1	15
3:B:147:HEC:HHD	2:D:42:PHE:HZ	0.60	1.56	15	1
1:A:24:TYR:CE1	1:A:112:HIS:CG	0.60	2.88	20	1
1:A:50:HIS:ND1	1:A:51:GLY:N	0.60	2.48	11	4
2:D:38:THR:HB	3:D:147:HEC:HBC1	0.60	1.73	6	1
1:C:112:HIS:CG	1:C:113:LEU:H	0.60	2.14	16	1
1:A:45:HIS:ND1	1:A:45:HIS:C	0.60	2.54	19	7
1:C:72:HIS:O	1:C:73:VAL:HG12	0.60	1.95	13	20
1:C:69:ALA:HB1	1:C:76:MET:SD	0.60	2.36	18	9
2:B:42:PHE:CE1	3:B:147:HEC:HMD3	0.60	2.31	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:67:VAL:CG2	3:B:147:HEC:NB	0.60	2.65	9	2
1:A:35:SER:HA	2:B:131:GLN:OE1	0.60	1.97	10	1
1:A:105:LEU:HD12	1:A:105:LEU:C	0.60	2.16	13	1
1:A:112:HIS:CG	1:A:113:LEU:N	0.60	2.68	16	1
2:D:56:GLY:O	2:D:57:ASN:CB	0.60	2.49	19	1
2:D:37:TRP:CZ2	2:D:102:ASN:ND2	0.60	2.70	5	1
2:D:31:LEU:HD23	2:D:31:LEU:O	0.60	1.97	9	1
2:B:40:ARG:HE	1:C:92:ARG:HH21	0.60	0.62	15	1
1:A:34:LEU:HD12	1:A:35:SER:N	0.60	2.11	1	4
1:C:80:LEU:N	1:C:80:LEU:HD12	0.60	2.12	18	2
2:B:139:ASN:HD22	2:D:139:ASN:ND2	0.60	1.94	3	1
2:B:38:THR:HB	3:B:147:HEC:HBC1	0.60	1.73	6	1
1:A:92:ARG:NE	2:D:40:ARG:CG	0.60	2.61	19	2
1:A:34:LEU:HD11	2:B:128:ALA:N	0.60	2.11	18	1
1:A:5:ALA:O	1:A:7:LYS:N	0.60	2.35	12	8
1:A:34:LEU:CB	2:B:128:ALA:HB2	0.60	2.23	15	1
1:C:101:LEU:HD12	3:C:142:HEC:C1C	0.60	2.27	19	1
2:D:3:LEU:HD13	2:D:8:LYS:HB3	0.60	1.73	6	6
1:C:129:LEU:C	1:C:129:LEU:HD12	0.60	2.17	6	1
1:A:33:PHE:O	1:A:36:PHE:CD2	0.60	2.55	3	2
1:A:120:ALA:O	1:A:124:SER:N	0.60	2.35	4	17
1:A:129:LEU:C	1:A:129:LEU:HD12	0.60	2.17	6	1
1:C:48:LEU:CD1	3:C:142:HEC:C1A	0.60	2.66	12	1
1:C:5:ALA:O	1:C:7:LYS:N	0.59	2.34	12	7
1:C:52:SER:O	1:C:53:ALA:HB3	0.59	1.96	3	13
1:A:113:LEU:O	1:A:113:LEU:CD2	0.59	2.50	1	2
1:A:121:VAL:CG1	1:A:122:HIS:N	0.59	2.65	13	18
1:C:33:PHE:O	1:C:36:PHE:CD2	0.59	2.55	3	2
2:B:146:HIS:HD2	2:D:135:ALA:O	0.59	1.72	17	1
2:B:17:LYS:CD	2:B:17:LYS:H	0.59	2.09	14	4
2:B:31:LEU:HD23	2:B:31:LEU:O	0.59	1.97	9	1
1:C:101:LEU:HD13	3:C:142:HEC:C1C	0.59	2.27	2	1
1:A:46:PHE:O	1:A:48:LEU:CD1	0.59	2.50	5	3
2:B:37:TRP:CZ2	2:B:102:ASN:ND2	0.59	2.70	5	1
1:C:40:LYS:O	3:C:142:HEC:ND	0.59	2.20	12	1
3:B:147:HEC:HHC	2:D:106:LEU:HD12	0.59	1.49	15	1
1:A:94:ASP:O	1:A:96:VAL:N	0.59	2.35	4	8
1:C:117:PHE:HE1	2:D:30:ARG:NH2	0.59	1.88	3	1
1:C:101:LEU:HB2	3:C:142:HEC:HMC3	0.59	1.73	2	2
1:C:35:SER:HA	2:D:131:GLN:OE1	0.59	1.97	10	1
1:C:94:ASP:O	1:C:96:VAL:N	0.59	2.35	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD13	3:A:142:HEC:C1C	0.59	2.27	2	1
1:A:97:ASN:HD22	1:A:97:ASN:N	0.59	1.95	9	2
1:C:97:ASN:N	1:C:97:ASN:HD22	0.59	1.95	9	2
1:C:34:LEU:CD1	2:D:128:ALA:N	0.59	2.66	18	1
1:C:113:LEU:O	1:C:113:LEU:CD2	0.59	2.50	1	1
2:B:106:LEU:HD21	3:B:147:HEC:CAB	0.59	2.28	2	1
2:B:97:HIS:ND1	2:B:97:HIS:C	0.59	2.56	14	3
2:D:3:LEU:N	2:D:3:LEU:CD1	0.59	2.64	8	12
2:D:93:CYS:SG	2:D:145:TYR:CD1	0.59	2.96	3	1
1:A:101:LEU:HD12	3:A:142:HEC:C1C	0.59	2.27	19	2
1:C:34:LEU:CB	2:D:128:ALA:HB2	0.59	2.23	15	1
1:A:122:HIS:NE2	2:B:112:CYS:SG	0.59	2.76	17	1
2:B:99:ASP:HB2	1:C:96:VAL:CG2	0.59	2.27	18	1
2:B:56:GLY:O	2:B:57:ASN:CB	0.59	2.49	19	1
1:C:7:LYS:N	1:C:7:LYS:CD	0.59	2.66	20	1
2:D:106:LEU:HD21	3:D:147:HEC:CAB	0.58	2.28	2	1
1:A:80:LEU:N	1:A:80:LEU:HD12	0.58	2.12	18	2
2:D:17:LYS:CD	2:D:17:LYS:H	0.58	2.09	14	4
2:B:30:ARG:NH2	2:B:55:MET:SD	0.58	2.77	9	1
2:D:82:LYS:NZ	2:D:143:HIS:CD2	0.58	2.71	20	2
1:C:122:HIS:NE2	2:D:112:CYS:SG	0.58	2.76	17	1
1:A:34:LEU:CD1	2:B:128:ALA:N	0.58	2.66	18	1
2:D:92:HIS:O	2:D:97:HIS:N	0.58	2.37	11	14
1:A:24:TYR:N	1:A:24:TYR:CD1	0.58	2.71	12	13
2:B:133:VAL:CG1	2:B:134:VAL:N	0.58	2.66	19	6
2:D:30:ARG:NH2	2:D:55:MET:SD	0.58	2.77	9	1
1:C:117:PHE:HE1	2:D:116:HIS:NE2	0.58	1.89	20	1
1:C:121:VAL:CG1	1:C:122:HIS:N	0.58	2.65	13	18
1:C:48:LEU:N	1:C:48:LEU:CD2	0.58	2.66	2	1
2:B:119:GLY:O	2:B:122:PHE:CD1	0.58	2.57	6	9
1:C:46:PHE:O	1:C:48:LEU:CD1	0.58	2.50	5	3
2:B:3:LEU:H	2:B:3:LEU:CD1	0.58	2.06	12	3
2:D:67:VAL:CG2	3:D:147:HEC:NB	0.58	2.64	9	2
2:B:117:HIS:CE1	2:B:118:PHE:CZ	0.58	2.92	10	1
2:D:117:HIS:CE1	2:D:118:PHE:CZ	0.58	2.92	10	1
2:B:97:HIS:N	2:B:97:HIS:CD2	0.58	2.72	15	1
1:A:7:LYS:N	1:A:7:LYS:CD	0.58	2.66	20	1
2:B:92:HIS:O	2:B:97:HIS:N	0.58	2.37	11	14
2:D:88:LEU:O	2:D:92:HIS:N	0.58	2.37	18	2
1:C:24:TYR:CG	1:C:112:HIS:NE2	0.58	2.72	7	1
2:D:2:HIS:CG	2:D:2:HIS:O	0.58	2.55	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:31:ARG:HH12	2:D:127:GLN:HB2	0.58	1.57	16	1
2:D:67:VAL:HG13	3:D:147:HEC:NB	0.58	2.06	19	1
1:A:96:VAL:HB	2:D:99:ASP:OD2	0.58	1.98	2	2
1:A:38:THR:HB	2:D:97:HIS:HB2	0.58	1.74	5	1
1:A:101:LEU:HD13	3:A:142:HEC:HBB3	0.58	1.76	15	1
1:A:92:ARG:HD3	2:D:40:ARG:HB3	0.58	1.76	17	1
1:C:7:LYS:O	1:C:10:VAL:N	0.58	2.36	20	11
1:A:48:LEU:CD2	1:A:48:LEU:N	0.58	2.66	2	1
1:A:86:LEU:HD21	3:A:142:HEC:CBD	0.58	2.29	12	4
2:B:82:LYS:NZ	2:B:143:HIS:CD2	0.58	2.71	20	2
1:A:92:ARG:O	1:A:93:VAL:O	0.58	2.21	13	2
2:B:2:HIS:CG	2:B:2:HIS:O	0.58	2.55	14	1
1:A:7:LYS:O	1:A:10:VAL:N	0.58	2.36	20	11
2:D:106:LEU:HB3	3:D:147:HEC:CAB	0.58	2.29	18	3
2:B:45:PHE:CZ	3:B:147:HEC:HMD3	0.58	2.34	16	1
2:D:75:LEU:N	2:D:75:LEU:CD2	0.58	2.67	20	3
2:D:92:HIS:NE2	2:D:141:LEU:O	0.58	2.37	5	3
1:C:58:HIS:O	1:C:58:HIS:ND1	0.58	2.36	10	5
2:B:41:PHE:CE2	3:B:147:HEC:CMD	0.58	2.86	12	1
2:D:39:GLN:HG2	3:D:147:HEC:CHC	0.58	2.06	12	1
1:C:92:ARG:O	1:C:93:VAL:O	0.58	2.21	13	2
2:D:45:PHE:CZ	3:D:147:HEC:HMD3	0.58	2.34	16	1
2:B:40:ARG:CD	1:C:92:ARG:NE	0.58	2.50	19	1
2:B:92:HIS:NE2	2:B:141:LEU:O	0.58	2.37	5	3
2:B:145:TYR:CG	2:B:145:TYR:O	0.58	2.57	12	2
1:A:24:TYR:CG	1:A:112:HIS:NE2	0.58	2.72	7	1
1:C:93:VAL:CG2	1:C:97:ASN:ND2	0.58	2.67	12	1
1:C:101:LEU:CD1	3:C:142:HEC:C1C	0.58	2.82	15	1
1:A:31:ARG:NH1	1:A:104:CYS:SG	0.57	2.77	2	1
2:D:133:VAL:CG1	2:D:134:VAL:N	0.57	2.66	19	5
1:A:92:ARG:O	2:D:40:ARG:NH1	0.57	2.36	14	1
2:B:40:ARG:NH2	1:C:93:VAL:O	0.57	2.37	14	1
2:D:146:HIS:HD1	2:D:146:HIS:H	0.57	1.41	17	1
2:B:139:ASN:ND2	2:D:139:ASN:HD22	0.57	1.93	3	1
1:A:45:HIS:O	1:A:45:HIS:ND1	0.57	2.37	20	10
1:A:36:PHE:CZ	2:B:104:ARG:NH2	0.57	2.73	5	1
2:D:97:HIS:O	2:D:97:HIS:ND1	0.57	2.38	6	4
1:C:35:SER:O	1:C:36:PHE:C	0.57	2.43	1	2
1:C:45:HIS:ND1	1:C:45:HIS:O	0.57	2.37	20	11
1:A:17:VAL:O	1:A:18:GLY:C	0.57	2.42	11	3
2:D:97:HIS:ND1	2:D:97:HIS:C	0.57	2.56	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:88:LEU:O	2:B:92:HIS:N	0.57	2.37	18	3
1:C:52:SER:O	1:C:53:ALA:HB2	0.57	1.99	14	3
2:D:30:ARG:NH2	2:D:55:MET:CE	0.57	2.67	9	1
2:D:114:LEU:HD12	2:D:114:LEU:N	0.57	2.14	9	1
1:A:61:LYS:HB3	3:A:142:HEC:C2A	0.57	2.30	14	9
2:B:93:CYS:SG	2:B:145:TYR:CD1	0.57	2.96	3	1
2:D:97:HIS:CD2	2:D:97:HIS:C	0.57	2.78	5	1
1:A:29:LEU:HD11	1:A:58:HIS:ND1	0.57	2.15	18	9
2:D:119:GLY:O	2:D:122:PHE:CD1	0.57	2.57	6	10
2:D:145:TYR:CG	2:D:145:TYR:O	0.57	2.57	12	1
2:B:135:ALA:HB1	2:D:146:HIS:OXT	0.57	1.98	18	1
1:A:92:ARG:NH2	2:D:37:TRP:O	0.57	2.38	19	1
2:D:57:ASN:N	2:D:58:PRO:HD3	0.57	2.13	19	1
1:A:52:SER:O	1:A:53:ALA:HB2	0.57	1.99	14	3
1:A:94:ASP:OD2	2:D:40:ARG:NH1	0.57	2.38	3	1
1:A:106:LEU:N	1:A:106:LEU:HD22	0.57	2.14	4	5
2:B:106:LEU:HB3	3:B:147:HEC:CAB	0.57	2.29	18	3
2:B:41:PHE:CE2	3:B:147:HEC:HMD1	0.57	2.35	12	1
1:C:50:HIS:ND1	1:C:50:HIS:N	0.57	2.53	1	3
1:C:45:HIS:O	1:C:45:HIS:CD2	0.57	2.58	2	2
1:C:24:TYR:CD1	1:C:24:TYR:N	0.57	2.71	12	17
2:D:37:TRP:CD1	2:D:38:THR:N	0.57	2.73	4	6
1:C:36:PHE:CZ	2:D:104:ARG:NH2	0.57	2.73	5	1
2:B:114:LEU:HD12	2:B:114:LEU:N	0.57	2.14	9	1
1:A:18:GLY:O	1:A:19:ALA:HB3	0.57	2.00	11	3
1:C:7:LYS:CD	1:C:7:LYS:H	0.57	2.11	20	1
1:C:29:LEU:HD11	1:C:58:HIS:ND1	0.57	2.15	18	9
1:C:31:ARG:NH1	1:C:104:CYS:SG	0.57	2.77	2	1
1:C:106:LEU:N	1:C:106:LEU:HD22	0.57	2.14	4	5
1:A:7:LYS:CD	1:A:7:LYS:H	0.57	2.12	20	1
1:A:41:THR:HG21	2:D:94:ASP:O	0.57	1.99	6	1
2:B:97:HIS:O	2:B:97:HIS:ND1	0.57	2.38	6	4
1:C:17:VAL:O	1:C:18:GLY:C	0.57	2.43	11	3
1:A:101:LEU:CD1	3:A:142:HEC:C1C	0.57	2.82	15	1
1:C:61:LYS:HB3	3:C:142:HEC:C2A	0.56	2.29	20	9
2:B:96:LEU:O	2:B:97:HIS:CB	0.56	2.53	5	6
2:D:96:LEU:O	2:D:97:HIS:CB	0.56	2.53	5	6
1:A:31:ARG:NH2	1:A:104:CYS:SG	0.56	2.79	7	1
1:A:58:HIS:O	1:A:58:HIS:ND1	0.56	2.36	10	5
2:B:30:ARG:NH2	2:B:55:MET:CE	0.56	2.68	9	1
1:A:93:VAL:CG2	1:A:97:ASN:ND2	0.56	2.67	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:106:LEU:HG	3:B:147:HEC:CHC	0.56	2.30	18	1
1:A:35:SER:O	1:A:36:PHE:C	0.56	2.43	1	2
1:A:50:HIS:ND1	1:A:50:HIS:N	0.56	2.53	1	4
1:C:34:LEU:O	1:C:36:PHE:CZ	0.56	2.58	1	1
2:B:38:THR:C	2:B:40:ARG:H	0.56	2.04	15	2
1:A:4:PRO:O	1:A:6:ASP:N	0.56	2.38	7	5
2:B:111:VAL:CG2	2:B:130:TYR:CE1	0.56	2.88	6	2
2:D:42:PHE:CA	3:D:147:HEC:CMA	0.56	2.79	12	1
2:B:28:LEU:HD12	2:B:28:LEU:N	0.56	2.15	18	2
1:A:34:LEU:O	1:A:36:PHE:CZ	0.56	2.58	1	1
2:B:84:THR:CG2	2:B:85:PHE:N	0.56	2.68	20	18
2:D:45:PHE:O	2:D:47:ASP:N	0.56	2.39	14	7
1:A:45:HIS:O	1:A:45:HIS:CD2	0.56	2.58	2	2
2:B:42:PHE:CD2	3:B:147:HEC:HMD3	0.56	2.32	2	1
2:B:146:HIS:CB	2:D:135:ALA:HB1	0.56	2.29	3	1
1:A:48:LEU:HD12	1:A:48:LEU:H	0.56	1.60	8	3
2:B:97:HIS:CD2	2:B:97:HIS:C	0.56	2.78	5	1
1:C:4:PRO:O	1:C:6:ASP:N	0.56	2.38	7	5
2:D:96:LEU:N	2:D:96:LEU:HD12	0.56	2.15	15	3
2:D:133:VAL:CG1	2:D:134:VAL:H	0.56	2.13	9	3
1:A:50:HIS:CG	1:A:51:GLY:N	0.56	2.73	11	1
1:A:92:ARG:HG2	2:D:40:ARG:NH1	0.56	2.16	14	1
1:A:93:VAL:O	2:D:40:ARG:NH2	0.56	2.38	14	1
1:C:101:LEU:HD13	3:C:142:HEC:HBB3	0.56	1.76	15	1
2:D:97:HIS:N	2:D:97:HIS:CD2	0.56	2.72	15	1
1:A:107:VAL:CG1	2:B:127:GLN:NE2	0.56	2.68	17	1
2:B:146:HIS:NE2	2:D:135:ALA:HB1	0.56	2.15	17	1
2:B:57:ASN:N	2:B:58:PRO:HD3	0.56	2.13	19	1
2:B:94:ASP:O	2:B:97:HIS:NE2	0.56	2.39	4	6
1:C:37:PRO:O	1:C:39:THR:N	0.56	2.39	10	9
2:B:75:LEU:N	2:B:75:LEU:CD2	0.56	2.66	20	3
1:C:34:LEU:O	1:C:36:PHE:CE2	0.56	2.59	1	1
1:C:20:HIS:O	1:C:24:TYR:CD2	0.56	2.59	1	1
2:D:122:PHE:CG	2:D:122:PHE:O	0.56	2.58	18	15
1:C:35:SER:O	1:C:36:PHE:CG	0.56	2.59	4	11
1:A:38:THR:HG22	2:D:97:HIS:O	0.56	2.01	3	1
2:D:76:ALA:O	2:D:77:HIS:CG	0.56	2.59	6	8
2:B:133:VAL:CG1	2:B:134:VAL:H	0.56	2.13	12	3
2:B:80:ASN:N	2:B:80:ASN:ND2	0.56	2.52	14	1
2:B:139:ASN:HD22	2:D:146:HIS:HE1	0.56	1.41	20	1
2:D:38:THR:C	2:D:40:ARG:H	0.56	2.04	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:48:LEU:H	1:C:48:LEU:HD12	0.56	1.60	8	3
1:C:31:ARG:NH2	1:C:104:CYS:SG	0.56	2.79	7	1
2:B:40:ARG:NH1	1:C:92:ARG:O	0.56	2.38	14	1
1:A:20:HIS:O	1:A:24:TYR:CD2	0.56	2.59	1	1
2:B:122:PHE:CG	2:B:122:PHE:O	0.56	2.58	16	15
2:D:84:THR:CG2	2:D:85:PHE:N	0.56	2.69	12	18
1:A:46:PHE:O	1:A:48:LEU:HD12	0.56	2.01	18	3
2:D:111:VAL:CG2	2:D:130:TYR:CE1	0.56	2.89	18	2
2:D:48:LEU:HD21	3:D:147:HEC:HMA3	0.56	1.77	12	1
2:D:80:ASN:ND2	2:D:80:ASN:N	0.56	2.52	14	1
2:D:28:LEU:N	2:D:28:LEU:HD12	0.56	2.15	18	2
1:A:34:LEU:O	1:A:36:PHE:CE2	0.56	2.59	1	1
2:B:45:PHE:O	2:B:47:ASP:N	0.56	2.39	14	7
1:A:95:PRO:O	1:A:98:PHE:CD2	0.56	2.58	13	1
1:C:95:PRO:O	1:C:98:PHE:CD2	0.56	2.59	13	1
1:C:129:LEU:HD22	3:C:142:HEC:HBB1	0.56	1.78	16	2
1:A:92:ARG:CZ	2:D:40:ARG:HG3	0.56	2.31	15	1
2:B:42:PHE:CE1	2:B:45:PHE:CE1	0.56	2.94	16	1
1:A:101:LEU:HD23	3:A:142:HEC:CAB	0.56	2.31	20	2
1:C:52:SER:O	1:C:54:GLN:N	0.55	2.39	18	7
1:A:37:PRO:O	1:A:39:THR:N	0.55	2.39	10	9
2:B:37:TRP:CD1	2:B:38:THR:N	0.55	2.73	4	6
1:C:50:HIS:CG	1:C:51:GLY:N	0.55	2.73	11	1
1:C:107:VAL:CG1	2:D:127:GLN:NE2	0.55	2.68	17	1
2:B:106:LEU:HG	3:B:147:HEC:C4B	0.55	2.30	18	1
2:D:19:ASN:O	2:D:21:ASP:N	0.55	2.40	16	15
2:D:38:THR:OG1	2:D:39:GLN:N	0.55	2.40	20	4
2:D:94:ASP:O	2:D:97:HIS:NE2	0.55	2.38	4	6
1:C:91:LEU:N	1:C:91:LEU:HD12	0.55	2.16	7	4
2:D:146:HIS:HD1	2:D:146:HIS:N	0.55	1.98	17	2
2:D:103:PHE:HA	3:D:147:HEC:HBB2	0.55	1.77	16	1
2:D:106:LEU:HG	3:D:147:HEC:C4B	0.55	2.30	18	1
2:B:19:ASN:O	2:B:21:ASP:N	0.55	2.40	16	15
2:D:45:PHE:HZ	3:D:147:HEC:CMD	0.55	2.15	16	1
2:B:132:LYS:HG3	2:D:146:HIS:HB3	0.55	1.77	19	1
1:A:35:SER:O	1:A:36:PHE:CG	0.55	2.59	4	12
1:A:94:ASP:CG	2:D:99:ASP:OD1	0.55	2.45	2	1
1:C:97:ASN:N	1:C:97:ASN:OD1	0.55	2.40	12	2
1:C:101:LEU:HD23	3:C:142:HEC:CAB	0.55	2.31	20	2
1:C:108:THR:CG2	1:C:109:LEU:N	0.55	2.69	16	2
1:C:113:LEU:O	1:C:114:PRO:O	0.55	2.25	18	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:N	1:A:91:LEU:HD12	0.55	2.16	7	4
2:B:96:LEU:N	2:B:96:LEU:HD12	0.55	2.15	15	3
3:B:147:HEC:CHA	2:D:63:HIS:HE1	0.55	2.13	15	1
2:B:103:PHE:HA	3:B:147:HEC:HBB2	0.55	1.77	16	1
3:C:142:HEC:HMB1	3:C:142:HEC:CBB	0.55	2.31	11	5
2:B:105:LEU:HD12	2:B:105:LEU:N	0.55	2.16	13	4
1:A:113:LEU:C	1:A:113:LEU:HD13	0.55	2.21	12	4
1:C:46:PHE:O	1:C:48:LEU:HD12	0.55	2.01	18	3
2:B:76:ALA:O	2:B:77:HIS:CG	0.55	2.59	6	8
2:B:40:ARG:CB	1:C:92:ARG:HE	0.55	1.89	19	2
1:C:111:ALA:HB2	2:D:122:PHE:CD2	0.55	2.30	8	2
2:B:66:LYS:HB3	3:B:147:HEC:HBA2	0.55	1.78	14	1
1:A:31:ARG:NH2	2:B:124:PRO:HA	0.55	2.17	15	1
2:D:63:HIS:HE1	3:D:147:HEC:CAA	0.55	2.14	16	1
2:B:146:HIS:OXT	2:D:135:ALA:HB1	0.55	2.02	18	1
1:A:52:SER:O	1:A:54:GLN:N	0.55	2.39	1	7
2:D:55:MET:SD	2:D:55:MET:N	0.55	2.80	6	6
2:B:40:ARG:NH1	1:C:94:ASP:OD2	0.55	2.40	3	1
1:C:113:LEU:C	1:C:113:LEU:HD13	0.55	2.21	12	4
1:A:111:ALA:HB2	2:B:122:PHE:CD2	0.55	2.30	8	2
1:A:61:LYS:HG2	3:A:142:HEC:HAA1	0.55	1.78	11	2
1:C:61:LYS:O	1:C:65:ALA:N	0.55	2.40	17	2
1:C:36:PHE:CB	3:C:142:HEC:CMC	0.55	2.82	12	1
2:B:63:HIS:HE1	3:B:147:HEC:CAA	0.55	2.14	16	1
2:D:106:LEU:HG	3:D:147:HEC:CHC	0.55	2.31	18	1
2:B:53:ALA:O	2:B:57:ASN:ND2	0.55	2.40	3	2
2:D:106:LEU:HD12	3:D:147:HEC:HMC3	0.55	1.79	17	3
2:B:97:HIS:HB2	1:C:38:THR:HB	0.55	1.79	5	1
1:C:18:GLY:O	1:C:19:ALA:HB3	0.55	2.00	11	3
2:D:103:PHE:N	2:D:103:PHE:CD1	0.55	2.73	11	1
1:A:31:ARG:HH12	2:B:127:GLN:HB2	0.55	1.57	16	1
2:D:63:HIS:CE1	3:D:147:HEC:C2A	0.55	2.90	16	1
1:C:101:LEU:CD2	3:C:142:HEC:CAB	0.55	2.85	20	5
2:D:105:LEU:N	2:D:105:LEU:HD12	0.55	2.16	13	5
1:A:106:LEU:N	1:A:106:LEU:CD2	0.55	2.70	20	6
1:C:106:LEU:N	1:C:106:LEU:CD2	0.55	2.70	5	6
2:D:3:LEU:H	2:D:3:LEU:CD1	0.55	2.12	20	4
2:D:37:TRP:NE1	2:D:38:THR:OG1	0.55	2.40	18	4
2:B:81:LEU:O	2:B:85:PHE:CZ	0.55	2.60	6	1
2:D:59:LYS:O	2:D:63:HIS:N	0.55	2.39	7	2
1:A:100:LEU:N	1:A:100:LEU:HD22	0.55	2.17	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:100:LEU:N	1:C:100:LEU:HD22	0.55	2.17	9	1
1:A:61:LYS:O	1:A:65:ALA:N	0.55	2.40	17	3
2:B:93:CYS:O	2:B:97:HIS:CD2	0.55	2.60	12	1
2:D:93:CYS:O	2:D:97:HIS:CD2	0.55	2.60	12	1
1:C:85:ASP:OD1	1:C:89:HIS:CE1	0.55	2.60	20	1
1:A:3:SER:O	1:A:4:PRO:O	0.55	2.25	3	3
1:C:3:SER:O	1:C:4:PRO:O	0.55	2.25	3	2
1:A:101:LEU:CD2	3:A:142:HEC:CAB	0.55	2.85	20	5
1:A:47:ASP:O	1:A:49:SER:N	0.55	2.40	19	10
2:D:13:ALA:O	2:D:15:TRP:N	0.55	2.40	15	3
2:B:73:ASP:CG	2:B:84:THR:HG1	0.55	2.05	15	1
2:D:45:PHE:CZ	3:D:147:HEC:CMD	0.55	2.90	16	1
2:B:42:PHE:O	2:B:44:SER:N	0.54	2.40	7	2
2:B:123:THR:OG1	2:B:126:VAL:HG23	0.54	2.03	18	8
2:D:81:LEU:N	2:D:81:LEU:CD2	0.54	2.71	10	2
2:D:42:PHE:CD1	3:D:147:HEC:CHB	0.54	2.90	12	1
1:A:129:LEU:HD22	3:A:142:HEC:HBB1	0.54	1.78	16	2
2:B:45:PHE:CZ	3:B:147:HEC:CMD	0.54	2.90	16	1
1:C:34:LEU:CD1	2:D:128:ALA:H	0.54	2.15	18	1
1:A:35:SER:O	1:A:36:PHE:CD2	0.54	2.61	19	6
2:D:42:PHE:O	2:D:44:SER:N	0.54	2.40	7	2
2:B:42:PHE:CD1	2:B:43:GLU:N	0.54	2.76	5	1
1:C:36:PHE:CD2	3:C:142:HEC:HMC1	0.54	2.36	12	1
1:C:36:PHE:CB	3:C:142:HEC:HMC1	0.54	2.33	12	1
1:A:92:ARG:CB	2:D:40:ARG:NH2	0.54	2.67	17	2
2:B:55:MET:SD	2:B:55:MET:N	0.54	2.80	6	6
1:A:95:PRO:O	1:A:97:ASN:N	0.54	2.41	6	10
2:B:146:HIS:HB3	2:D:135:ALA:HB1	0.54	1.77	3	1
2:B:106:LEU:HD12	3:B:147:HEC:HMC3	0.54	1.79	17	3
1:C:32:MET:O	1:C:36:PHE:N	0.54	2.40	7	1
1:C:61:LYS:HG2	3:C:142:HEC:HAA1	0.54	1.78	11	3
1:A:116:GLU:O	1:A:117:PHE:CG	0.54	2.60	14	2
1:C:31:ARG:NH2	2:D:124:PRO:HA	0.54	2.17	15	1
2:D:81:LEU:N	2:D:81:LEU:HD22	0.54	2.17	15	1
2:B:142:ALA:O	2:B:145:TYR:CD1	0.54	2.61	16	2
1:C:123:ALA:HB2	2:D:34:VAL:HA	0.54	1.79	20	1
1:A:65:ALA:O	1:A:69:ALA:N	0.54	2.40	12	5
1:A:86:LEU:CG	3:A:142:HEC:HBD1	0.54	2.32	7	1
1:C:100:LEU:N	1:C:100:LEU:CD2	0.54	2.71	9	1
1:A:109:LEU:O	1:A:112:HIS:NE2	0.54	2.41	16	1
2:D:42:PHE:CE1	2:D:45:PHE:CE1	0.54	2.95	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:CD1	2:B:128:ALA:H	0.54	2.15	18	1
1:C:98:PHE:CG	1:C:99:LYS:N	0.54	2.75	19	1
2:B:116:HIS:ND1	2:B:116:HIS:C	0.54	2.61	18	15
1:A:113:LEU:O	1:A:114:PRO:O	0.54	2.25	18	12
2:D:53:ALA:O	2:D:57:ASN:ND2	0.54	2.40	3	2
2:B:37:TRP:NE1	2:B:38:THR:OG1	0.54	2.41	9	4
2:D:42:PHE:CD1	2:D:43:GLU:N	0.54	2.76	5	1
1:C:86:LEU:CG	3:C:142:HEC:HBD1	0.54	2.32	7	1
2:D:94:ASP:O	2:D:97:HIS:CD2	0.54	2.61	9	2
1:A:101:LEU:HD23	1:A:101:LEU:O	0.54	2.02	13	2
1:C:101:LEU:HD23	1:C:101:LEU:O	0.54	2.02	13	2
2:B:40:ARG:NH1	1:C:92:ARG:HG2	0.54	2.17	14	1
2:B:81:LEU:N	2:B:81:LEU:HD22	0.54	2.17	15	1
2:D:73:ASP:CG	2:D:84:THR:HG1	0.54	2.05	15	1
2:B:45:PHE:HZ	3:B:147:HEC:CMD	0.54	2.15	16	1
1:A:108:THR:CG2	1:A:109:LEU:N	0.54	2.69	16	2
1:A:124:SER:OG	1:A:125:LEU:N	0.54	2.41	3	8
2:B:11:VAL:HG23	2:B:130:TYR:CD2	0.54	2.38	15	4
1:C:127:LYS:O	1:C:130:ALA:N	0.54	2.39	17	12
1:A:97:ASN:N	1:A:97:ASN:ND2	0.54	2.55	9	2
2:D:94:ASP:O	2:D:97:HIS:CE1	0.54	2.61	12	2
2:B:97:HIS:CE1	1:C:41:THR:CB	0.54	2.91	12	1
1:A:92:ARG:CZ	2:D:40:ARG:CG	0.54	2.85	15	1
2:B:2:HIS:NE2	2:D:146:HIS:CG	0.54	2.62	15	1
2:B:63:HIS:CE1	3:B:147:HEC:C2A	0.54	2.90	16	1
1:A:89:HIS:O	1:A:89:HIS:ND1	0.54	2.41	17	1
2:B:47:ASP:O	2:B:48:LEU:CB	0.54	2.54	20	1
1:C:72:HIS:C	1:C:74:ASP:N	0.54	2.61	19	20
1:C:95:PRO:O	1:C:97:ASN:N	0.54	2.41	6	9
1:C:47:ASP:O	1:C:49:SER:N	0.54	2.40	19	10
1:A:101:LEU:HD11	3:A:142:HEC:CHC	0.54	2.32	7	1
2:B:59:LYS:O	2:B:63:HIS:N	0.54	2.39	7	2
2:B:94:ASP:O	2:B:97:HIS:CE1	0.54	2.61	12	2
1:A:97:ASN:N	1:A:97:ASN:OD1	0.54	2.40	12	2
1:A:100:LEU:CD1	1:A:100:LEU:N	0.54	2.71	15	1
1:A:92:ARG:HD3	2:D:40:ARG:CB	0.54	2.32	17	1
2:B:143:HIS:O	2:B:146:HIS:CG	0.54	2.60	18	1
2:D:143:HIS:O	2:D:146:HIS:CG	0.54	2.60	18	1
1:A:85:ASP:OD1	1:A:89:HIS:CE1	0.54	2.60	20	1
1:A:72:HIS:C	1:A:74:ASP:N	0.54	2.61	16	20
1:A:37:PRO:O	1:A:40:LYS:N	0.54	2.39	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:46:PHE:O	1:C:48:LEU:HG	0.54	2.03	14	4
2:D:37:TRP:CH2	2:D:102:ASN:ND2	0.54	2.76	5	1
2:D:81:LEU:O	2:D:85:PHE:CZ	0.54	2.60	6	1
1:C:11:LYS:O	1:C:15:GLY:N	0.54	2.41	20	2
1:C:34:LEU:HD11	2:D:127:GLN:NE2	0.54	2.18	9	1
2:D:115:ALA:O	2:D:119:GLY:N	0.54	2.41	9	2
1:A:87:HIS:NE2	3:A:142:HEC:ND	0.54	2.55	12	1
2:B:13:ALA:O	2:B:15:TRP:N	0.54	2.41	14	3
2:D:66:LYS:HB3	3:D:147:HEC:HBA2	0.54	1.78	14	1
1:A:100:LEU:N	1:A:100:LEU:HD12	0.54	2.18	15	1
1:A:38:THR:HB	2:D:97:HIS:CB	0.54	2.31	19	1
1:C:61:LYS:CB	3:C:142:HEC:C3A	0.54	2.83	19	1
1:C:31:ARG:O	1:C:31:ARG:NE	0.54	2.41	1	1
1:C:48:LEU:H	1:C:48:LEU:CD2	0.54	2.13	3	2
2:D:89:SER:O	2:D:93:CYS:N	0.54	2.41	2	1
2:D:123:THR:OG1	2:D:126:VAL:HG23	0.54	2.03	18	7
1:A:32:MET:O	1:A:36:PHE:N	0.54	2.40	7	1
1:A:86:LEU:CD1	3:A:142:HEC:HBD1	0.54	2.32	7	1
2:B:115:ALA:O	2:B:119:GLY:N	0.54	2.41	9	2
1:C:97:ASN:HD22	1:C:97:ASN:H	0.54	1.45	9	1
2:B:81:LEU:N	2:B:81:LEU:CD2	0.54	2.71	10	2
1:C:109:LEU:O	1:C:112:HIS:NE2	0.54	2.41	16	1
2:B:37:TRP:O	1:C:92:ARG:NH2	0.54	2.41	19	1
1:A:123:ALA:HB2	2:B:34:VAL:HA	0.54	1.79	20	1
1:A:91:LEU:O	1:A:93:VAL:N	0.54	2.41	12	7
1:C:68:ASN:O	1:C:72:HIS:CD2	0.54	2.61	11	2
1:C:91:LEU:O	1:C:93:VAL:N	0.54	2.41	3	7
1:A:134:THR:O	1:A:138:SER:N	0.54	2.41	9	2
1:C:124:SER:OG	1:C:125:LEU:N	0.54	2.41	3	8
2:D:116:HIS:ND1	2:D:116:HIS:C	0.54	2.61	18	14
1:A:46:PHE:O	1:A:48:LEU:HG	0.54	2.03	14	5
2:B:37:TRP:CH2	2:B:102:ASN:ND2	0.54	2.76	5	1
1:A:68:ASN:O	1:A:72:HIS:CD2	0.53	2.61	11	2
1:C:91:LEU:C	1:C:93:VAL:H	0.53	2.06	17	4
2:B:38:THR:OG1	2:B:39:GLN:N	0.53	2.41	3	4
1:A:33:PHE:O	1:A:33:PHE:CD1	0.53	2.62	5	3
1:A:11:LYS:O	1:A:15:GLY:N	0.53	2.41	20	2
1:A:83:LEU:HD22	3:A:142:HEC:HBA1	0.53	1.79	9	2
2:D:142:ALA:O	2:D:145:TYR:CD1	0.53	2.61	16	2
1:A:92:ARG:HD3	2:D:40:ARG:CG	0.53	2.32	17	1
1:A:98:PHE:CG	1:A:99:LYS:N	0.53	2.75	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:46:GLY:O	2:D:48:LEU:N	0.53	2.41	19	1
1:A:35:SER:O	1:A:36:PHE:CD1	0.53	2.61	5	8
1:C:35:SER:O	1:C:36:PHE:CD1	0.53	2.62	5	7
1:C:100:LEU:N	1:C:100:LEU:CD1	0.53	2.71	15	3
1:A:21:ALA:O	1:A:23:GLU:N	0.53	2.42	5	16
1:C:35:SER:O	1:C:36:PHE:CD2	0.53	2.61	19	6
1:C:33:PHE:CD1	1:C:33:PHE:O	0.53	2.62	5	3
2:B:81:LEU:N	2:B:81:LEU:HD12	0.53	2.18	11	6
2:B:94:ASP:O	2:B:97:HIS:CD2	0.53	2.61	9	2
1:A:97:ASN:HD22	1:A:97:ASN:H	0.53	1.45	9	1
1:C:17:VAL:O	1:C:20:HIS:N	0.53	2.40	16	3
1:A:36:PHE:CE2	1:A:38:THR:OG1	0.53	2.61	12	1
3:B:147:HEC:HAD2	2:D:63:HIS:NE2	0.53	2.17	15	1
1:C:123:ALA:HB2	2:D:33:VAL:O	0.53	2.04	17	1
1:C:58:HIS:ND1	1:C:58:HIS:C	0.53	2.62	8	15
1:A:30:GLU:OE1	1:A:50:HIS:ND1	0.53	2.41	2	1
2:B:105:LEU:N	2:B:105:LEU:CD1	0.53	2.72	13	4
2:B:39:GLN:O	2:B:42:PHE:CD1	0.53	2.62	14	3
2:B:92:HIS:ND1	2:B:93:CYS:N	0.53	2.56	20	2
2:D:92:HIS:CE1	2:D:141:LEU:O	0.53	2.62	5	2
1:A:97:ASN:OD1	1:A:98:PHE:N	0.53	2.41	8	1
2:D:101:GLU:OE1	2:D:101:GLU:N	0.53	2.42	8	1
2:B:139:ASN:OD1	2:D:139:ASN:OD1	0.53	2.25	13	1
2:D:11:VAL:HG23	2:D:130:TYR:CD2	0.53	2.38	15	2
2:B:2:HIS:O	2:B:2:HIS:CD2	0.53	2.61	14	1
1:C:116:GLU:O	1:C:117:PHE:CG	0.53	2.60	14	2
1:A:27:GLU:OE1	1:A:27:GLU:N	0.53	2.41	15	1
2:B:7:GLU:N	2:B:7:GLU:OE1	0.53	2.42	15	2
2:B:42:PHE:CE2	2:B:45:PHE:CG	0.53	2.97	16	1
1:C:89:HIS:ND1	1:C:89:HIS:O	0.53	2.41	17	1
2:B:127:GLN:N	2:B:127:GLN:OE1	0.53	2.42	20	1
1:C:21:ALA:O	1:C:23:GLU:N	0.53	2.42	5	16
1:C:90:LYS:O	1:C:92:ARG:N	0.53	2.42	16	3
1:C:35:SER:OG	1:C:36:PHE:CD2	0.53	2.62	7	1
2:D:95:LYS:O	2:D:97:HIS:CE1	0.53	2.61	9	1
1:A:27:GLU:OE2	1:A:112:HIS:NE2	0.53	2.41	10	2
2:D:100:PRO:O	2:D:102:ASN:N	0.53	2.41	10	1
2:B:106:LEU:HB3	3:B:147:HEC:CBB	0.53	2.34	18	1
2:D:47:ASP:O	2:D:48:LEU:CB	0.53	2.54	20	1
1:C:134:THR:O	1:C:138:SER:N	0.53	2.41	9	2
2:B:131:GLN:H	2:B:131:GLN:NE2	0.53	2.02	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:81:LEU:N	2:D:81:LEU:HD12	0.53	2.18	11	6
1:A:100:LEU:N	1:A:100:LEU:CD2	0.53	2.71	9	1
2:B:95:LYS:O	2:B:97:HIS:CE1	0.53	2.61	9	1
2:B:122:PHE:O	2:B:127:GLN:NE2	0.53	2.42	11	1
1:C:36:PHE:CE2	1:C:38:THR:OG1	0.53	2.61	12	1
1:C:2:LEU:N	1:C:2:LEU:HD22	0.53	2.18	19	1
2:D:117:HIS:O	2:D:118:PHE:CD1	0.53	2.62	3	6
1:C:37:PRO:O	1:C:40:LYS:N	0.53	2.39	14	4
2:D:81:LEU:N	2:D:81:LEU:CD1	0.53	2.72	11	4
1:A:34:LEU:HD11	2:B:127:GLN:NE2	0.53	2.18	9	1
2:D:133:VAL:O	2:D:135:ALA:N	0.53	2.42	12	1
2:B:105:LEU:CD1	2:B:105:LEU:N	0.53	2.72	18	1
1:A:2:LEU:HD22	1:A:2:LEU:N	0.53	2.18	19	1
2:D:15:TRP:HE1	2:D:72:SER:CB	0.53	2.17	9	5
2:B:99:ASP:OD2	1:C:96:VAL:HB	0.53	2.04	2	2
1:C:26:ALA:HB1	1:C:55:VAL:O	0.53	2.04	8	2
2:B:92:HIS:CE1	2:B:141:LEU:O	0.53	2.62	5	2
2:B:81:LEU:N	2:B:81:LEU:CD1	0.53	2.72	11	4
1:A:33:PHE:CE2	1:A:48:LEU:O	0.53	2.62	13	1
2:D:2:HIS:O	2:D:2:HIS:CD2	0.53	2.62	14	1
2:B:40:ARG:CD	1:C:92:ARG:NH2	0.53	2.69	15	1
1:C:27:GLU:OE1	1:C:27:GLU:N	0.53	2.41	15	1
2:B:105:LEU:N	2:B:105:LEU:HD12	0.53	2.17	18	1
2:D:106:LEU:HB3	3:D:147:HEC:CBB	0.53	2.34	18	1
2:B:46:GLY:O	2:B:48:LEU:N	0.53	2.41	19	1
1:A:31:ARG:O	1:A:31:ARG:NE	0.53	2.41	1	1
2:D:57:ASN:OD1	2:D:59:LYS:N	0.53	2.42	1	1
1:A:52:SER:OG	1:A:53:ALA:N	0.53	2.42	9	2
2:D:105:LEU:N	2:D:105:LEU:CD1	0.53	2.72	18	5
1:A:38:THR:HA	2:D:97:HIS:CB	0.53	2.29	4	1
2:D:22:GLU:O	2:D:25:GLY:N	0.53	2.42	20	3
2:D:80:ASN:OD1	2:D:80:ASN:N	0.53	2.42	6	3
1:A:94:ASP:N	1:A:94:ASP:OD1	0.53	2.42	9	3
2:D:139:ASN:O	2:D:143:HIS:N	0.53	2.42	16	3
1:C:83:LEU:HD22	3:C:142:HEC:HBA1	0.53	1.79	9	2
2:D:77:HIS:CE1	2:D:80:ASN:OD1	0.53	2.62	10	1
1:A:2:LEU:N	1:A:2:LEU:CD2	0.53	2.72	19	1
1:A:34:LEU:HD12	1:A:34:LEU:C	0.53	2.24	1	1
1:A:58:HIS:ND1	1:A:58:HIS:C	0.53	2.62	8	15
2:B:15:TRP:HE1	2:B:72:SER:CB	0.53	2.17	9	5
2:B:88:LEU:O	2:B:92:HIS:ND1	0.53	2.42	19	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:103:PHE:N	2:B:103:PHE:CD1	0.53	2.73	11	2
1:C:73:VAL:O	1:C:73:VAL:HG22	0.53	2.04	15	19
2:D:50:THR:O	2:D:53:ALA:N	0.53	2.41	11	8
1:C:83:LEU:O	1:C:86:LEU:N	0.53	2.42	4	2
1:A:27:GLU:OE1	1:A:112:HIS:NE2	0.53	2.42	3	3
1:A:83:LEU:O	1:A:87:HIS:ND1	0.53	2.42	14	3
1:C:27:GLU:OE1	1:C:112:HIS:NE2	0.53	2.42	3	3
2:D:39:GLN:O	2:D:42:PHE:CD1	0.53	2.62	14	3
2:D:92:HIS:ND1	2:D:93:CYS:N	0.53	2.56	20	2
1:C:97:ASN:N	1:C:97:ASN:ND2	0.53	2.56	9	3
2:B:139:ASN:O	2:B:143:HIS:N	0.53	2.42	8	3
2:B:117:HIS:O	2:B:118:PHE:CG	0.53	2.62	9	4
2:D:96:LEU:N	2:D:96:LEU:CD1	0.53	2.71	15	3
2:D:117:HIS:O	2:D:118:PHE:CG	0.53	2.62	9	4
2:B:146:HIS:OXT	2:B:146:HIS:CG	0.53	2.62	11	1
2:D:146:HIS:OXT	2:D:146:HIS:CG	0.53	2.62	11	1
1:A:35:SER:OG	2:B:131:GLN:NE2	0.53	2.38	14	1
1:C:122:HIS:CD2	2:D:34:VAL:HG22	0.53	2.39	14	1
1:A:92:ARG:CB	2:D:40:ARG:NH1	0.53	2.37	17	1
2:B:71:PHE:CD1	2:B:71:PHE:O	0.53	2.62	17	1
1:A:24:TYR:CD1	1:A:112:HIS:ND1	0.53	2.77	18	1
1:C:24:TYR:CD1	1:C:112:HIS:ND1	0.53	2.77	18	1
2:D:95:LYS:O	2:D:97:HIS:NE2	0.53	2.42	19	1
2:B:112:CYS:O	2:B:116:HIS:ND1	0.53	2.41	3	2
2:D:42:PHE:CD2	3:D:147:HEC:HMD3	0.53	2.32	2	1
1:A:67:THR:O	1:A:71:ALA:N	0.53	2.42	6	6
2:B:127:GLN:O	2:B:131:GLN:NE2	0.53	2.42	5	2
1:C:86:LEU:CD1	3:C:142:HEC:HBD1	0.53	2.32	7	1
2:D:144:LYS:O	2:D:146:HIS:N	0.53	2.43	16	6
1:C:27:GLU:OE2	1:C:112:HIS:NE2	0.53	2.41	10	2
1:C:33:PHE:CE2	1:C:48:LEU:O	0.53	2.62	13	1
2:D:71:PHE:O	2:D:71:PHE:CD1	0.53	2.62	17	2
2:D:146:HIS:N	2:D:146:HIS:ND1	0.53	2.56	17	1
1:A:45:HIS:ND1	1:A:45:HIS:O	0.52	2.42	1	3
1:A:127:LYS:O	1:A:130:ALA:N	0.52	2.39	17	11
1:C:52:SER:OG	1:C:53:ALA:N	0.52	2.42	9	2
1:C:82:ALA:O	1:C:85:ASP:N	0.52	2.42	11	19
2:D:68:LEU:HD23	2:D:68:LEU:C	0.52	2.24	4	1
1:C:107:VAL:O	1:C:110:ALA:HB3	0.52	2.04	5	5
2:D:131:GLN:NE2	2:D:131:GLN:H	0.52	2.02	5	1
2:D:77:HIS:NE2	2:D:80:ASN:OD1	0.52	2.42	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:6:ASP:OD2	1:C:127:LYS:NZ	0.52	2.42	10	1
2:B:133:VAL:O	2:B:135:ALA:N	0.52	2.41	12	1
1:C:84:SER:O	1:C:88:ALA:N	0.52	2.42	13	1
2:D:7:GLU:N	2:D:7:GLU:OE1	0.52	2.42	15	2
1:A:61:LYS:CB	3:A:142:HEC:C3A	0.52	2.83	19	1
2:B:50:THR:O	2:B:53:ALA:N	0.52	2.41	11	7
2:B:80:ASN:OD1	2:B:83:GLY:N	0.52	2.42	11	6
1:A:71:ALA:O	1:A:72:HIS:CD2	0.52	2.62	17	4
1:C:106:LEU:CD1	1:C:106:LEU:N	0.52	2.73	3	2
2:D:19:ASN:O	2:D:22:GLU:N	0.52	2.42	9	8
1:C:94:ASP:N	1:C:94:ASP:OD1	0.52	2.42	9	3
1:C:61:LYS:O	3:C:142:HEC:HMA3	0.52	2.05	9	3
1:C:97:ASN:OD1	1:C:98:PHE:N	0.52	2.41	8	1
2:D:61:LYS:O	2:D:65:LYS:NZ	0.52	2.42	9	3
1:A:6:ASP:OD2	1:A:127:LYS:NZ	0.52	2.42	10	1
2:B:77:HIS:CE1	2:B:80:ASN:OD1	0.52	2.62	10	1
2:D:89:SER:O	2:D:93:CYS:SG	0.52	2.67	10	3
2:B:114:LEU:CD1	2:B:130:TYR:CZ	0.52	2.92	12	2
2:D:28:LEU:N	2:D:28:LEU:CD2	0.52	2.73	13	2
1:C:115:ALA:CB	1:C:122:HIS:CE1	0.52	2.93	16	1
2:D:42:PHE:CE2	2:D:45:PHE:CG	0.52	2.97	16	1
1:A:123:ALA:HB2	2:B:33:VAL:O	0.52	2.04	17	1
2:B:145:TYR:CD2	2:B:145:TYR:O	0.52	2.62	17	1
1:A:32:MET:HE1	3:A:142:HEC:HBC2	0.52	1.81	19	1
2:B:95:LYS:O	2:B:97:HIS:NE2	0.52	2.42	19	1
1:C:2:LEU:N	1:C:2:LEU:CD2	0.52	2.72	19	1
2:D:88:LEU:O	2:D:92:HIS:ND1	0.52	2.42	19	6
1:A:6:ASP:OD1	1:A:6:ASP:N	0.52	2.42	4	3
2:B:61:LYS:NZ	2:B:61:LYS:CB	0.52	2.72	6	2
2:D:61:LYS:NZ	2:D:61:LYS:CB	0.52	2.72	6	2
1:C:2:LEU:HD13	1:C:131:SER:OG	0.52	2.05	5	1
1:A:91:LEU:N	1:A:91:LEU:CD1	0.52	2.72	7	4
2:B:77:HIS:NE2	2:B:80:ASN:OD1	0.52	2.42	7	1
2:B:144:LYS:O	2:B:146:HIS:N	0.52	2.42	19	6
1:C:39:THR:CA	3:C:142:HEC:C3C	0.52	2.79	12	1
1:A:92:ARG:HB2	2:D:40:ARG:NH2	0.52	2.20	18	1
1:A:18:GLY:O	1:A:20:HIS:N	0.52	2.41	17	14
2:B:122:PHE:CD1	2:B:122:PHE:C	0.52	2.82	8	15
1:A:53:ALA:O	1:A:55:VAL:N	0.52	2.42	2	5
1:C:30:GLU:OE1	1:C:50:HIS:ND1	0.52	2.41	2	1
1:C:71:ALA:O	1:C:72:HIS:CD2	0.52	2.62	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:LEU:HD23	2:B:68:LEU:C	0.52	2.24	4	1
1:C:6:ASP:N	1:C:6:ASP:OD1	0.52	2.42	4	2
1:A:93:VAL:CG1	1:A:94:ASP:N	0.52	2.73	18	2
1:C:91:LEU:N	1:C:91:LEU:CD1	0.52	2.72	7	4
2:B:61:LYS:O	2:B:65:LYS:NZ	0.52	2.42	9	3
2:D:145:TYR:CE1	2:D:146:HIS:OXT	0.52	2.63	10	1
1:A:92:ARG:NH1	2:D:40:ARG:C	0.52	2.62	17	1
2:B:40:ARG:NH1	1:C:92:ARG:CB	0.52	2.35	17	1
1:A:91:LEU:C	1:A:93:VAL:H	0.52	2.06	17	4
1:A:37:PRO:O	2:D:97:HIS:ND1	0.52	2.43	3	1
1:A:95:PRO:O	1:A:98:PHE:N	0.52	2.41	4	7
1:C:65:ALA:O	1:C:69:ALA:N	0.52	2.40	12	6
1:C:130:ALA:O	1:C:134:THR:N	0.52	2.43	7	2
2:D:30:ARG:O	2:D:33:VAL:N	0.52	2.43	9	2
1:C:87:HIS:NE2	1:C:136:LEU:O	0.52	2.42	10	1
2:D:91:LEU:HD23	2:D:92:HIS:N	0.52	2.20	12	1
1:C:121:VAL:CG1	1:C:122:HIS:H	0.52	2.18	13	3
1:C:35:SER:OG	2:D:131:GLN:NE2	0.52	2.38	14	1
1:A:48:LEU:H	1:A:48:LEU:CD2	0.52	2.12	3	2
2:B:3:LEU:HD21	2:B:133:VAL:HG22	0.52	1.81	15	3
2:D:127:GLN:OE1	2:D:127:GLN:N	0.52	2.41	20	2
1:A:5:ALA:O	1:A:8:THR:N	0.52	2.42	7	4
1:A:82:ALA:O	1:A:85:ASP:N	0.52	2.42	11	17
1:A:86:LEU:HG	3:A:142:HEC:HBD1	0.52	1.82	7	1
1:C:31:ARG:CZ	1:C:104:CYS:SG	0.52	2.98	7	1
2:B:96:LEU:N	2:B:96:LEU:CD1	0.52	2.72	15	3
2:B:100:PRO:O	2:B:102:ASN:ND2	0.52	2.43	9	1
2:D:122:PHE:O	2:D:127:GLN:NE2	0.52	2.42	11	1
2:D:42:PHE:CD1	3:D:147:HEC:CMB	0.52	2.91	12	1
2:D:114:LEU:CD1	2:D:130:TYR:CZ	0.52	2.92	12	2
2:B:28:LEU:N	2:B:28:LEU:CD2	0.52	2.73	13	2
2:B:39:GLN:O	2:B:42:PHE:CE1	0.52	2.63	14	1
2:B:146:HIS:N	2:B:146:HIS:ND1	0.52	2.56	17	1
1:C:5:ALA:O	1:C:8:THR:N	0.52	2.42	7	4
2:B:117:HIS:O	2:B:118:PHE:CD1	0.52	2.62	3	6
2:D:128:ALA:O	2:D:132:LYS:NZ	0.52	2.43	3	1
1:A:31:ARG:NH2	2:B:127:GLN:CB	0.52	2.73	4	1
1:A:130:ALA:O	1:A:134:THR:N	0.52	2.43	7	2
1:C:68:ASN:OD1	1:C:69:ALA:N	0.52	2.43	9	1
1:C:103:HIS:HB3	2:D:108:ASN:HD21	0.52	1.65	10	1
2:D:145:TYR:O	2:D:145:TYR:CD2	0.52	2.62	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:SER:O	1:A:88:ALA:N	0.52	2.42	13	1
1:A:122:HIS:CD2	2:B:34:VAL:HG22	0.52	2.39	14	1
2:B:42:PHE:CZ	2:B:45:PHE:CE2	0.52	2.98	16	1
2:D:145:TYR:CD1	2:D:146:HIS:N	0.52	2.77	16	2
1:A:92:ARG:NE	2:D:40:ARG:CD	0.52	2.54	19	1
1:A:92:ARG:NH1	2:D:43:GLU:OE2	0.52	2.42	20	1
1:A:73:VAL:HG22	1:A:73:VAL:O	0.52	2.04	15	19
1:A:97:ASN:O	1:A:100:LEU:N	0.52	2.41	1	1
2:B:77:HIS:CE1	2:B:79:ASP:OD2	0.52	2.63	1	1
1:C:90:LYS:C	1:C:92:ARG:H	0.52	2.08	3	3
2:D:32:LEU:O	2:D:36:PRO:N	0.52	2.43	1	4
1:A:127:LYS:CD	1:A:128:PHE:N	0.52	2.73	6	6
1:A:90:LYS:O	1:A:92:ARG:N	0.52	2.42	16	4
2:D:21:ASP:OD1	2:D:22:GLU:N	0.52	2.42	3	2
2:D:41:PHE:O	2:D:43:GLU:N	0.52	2.43	3	1
2:D:127:GLN:O	2:D:131:GLN:NE2	0.52	2.42	5	2
1:A:98:PHE:CE1	1:A:102:SER:OG	0.52	2.63	7	1
1:C:76:MET:N	1:C:77:PRO:HD2	0.52	2.20	13	4
1:C:39:THR:C	3:C:142:HEC:C1C	0.52	2.76	12	1
2:D:39:GLN:O	2:D:42:PHE:CE1	0.52	2.63	14	1
1:A:115:ALA:CB	1:A:122:HIS:CE1	0.52	2.93	16	1
2:D:77:HIS:CE1	2:D:79:ASP:OD2	0.52	2.63	1	1
2:D:122:PHE:CD1	2:D:122:PHE:C	0.52	2.83	7	15
2:B:89:SER:O	2:B:93:CYS:N	0.52	2.41	2	1
2:D:112:CYS:O	2:D:116:HIS:ND1	0.52	2.41	3	2
1:A:106:LEU:CD1	1:A:106:LEU:N	0.52	2.73	3	1
2:B:41:PHE:O	2:B:43:GLU:N	0.52	2.43	3	1
1:A:2:LEU:HD21	1:A:131:SER:OG	0.52	2.05	6	2
2:B:101:GLU:OE1	2:B:101:GLU:N	0.52	2.42	8	1
2:D:117:HIS:HD1	2:D:117:HIS:N	0.52	2.03	12	1
3:B:147:HEC:HAB	2:D:106:LEU:CD2	0.52	2.29	15	1
2:B:57:ASN:OD1	2:B:59:LYS:N	0.52	2.42	1	1
1:C:18:GLY:O	1:C:20:HIS:N	0.52	2.41	17	13
1:C:32:MET:CE	3:C:142:HEC:CBC	0.52	2.88	5	4
1:C:53:ALA:O	1:C:55:VAL:N	0.52	2.43	2	5
1:C:127:LYS:CD	1:C:128:PHE:N	0.52	2.73	6	6
1:C:2:LEU:HD21	1:C:131:SER:OG	0.52	2.05	6	2
1:C:10:VAL:HG21	1:C:128:PHE:CD2	0.52	2.40	10	3
1:A:38:THR:HG22	2:D:97:HIS:CG	0.52	2.35	7	1
2:D:42:PHE:CE1	2:D:45:PHE:CD2	0.52	2.98	8	1
2:B:143:HIS:CG	2:B:143:HIS:O	0.52	2.63	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:143:HIS:CG	2:D:143:HIS:O	0.52	2.63	10	1
1:A:41:THR:HG22	2:D:97:HIS:CE1	0.52	2.40	11	1
1:A:121:VAL:CG1	1:A:122:HIS:H	0.52	2.18	17	3
2:D:111:VAL:CG2	2:D:130:TYR:CD1	0.52	2.93	18	1
1:C:67:THR:O	1:C:71:ALA:N	0.51	2.42	6	6
1:C:103:HIS:CD2	2:D:108:ASN:OD1	0.51	2.63	5	2
1:A:68:ASN:OD1	1:A:69:ALA:N	0.51	2.43	9	1
2:B:89:SER:O	2:B:93:CYS:SG	0.51	2.67	10	3
2:B:139:ASN:OD1	2:B:139:ASN:N	0.51	2.42	17	2
1:A:92:ARG:HB3	2:D:40:ARG:NE	0.51	2.19	18	1
1:A:61:LYS:HB3	3:A:142:HEC:C4A	0.51	2.35	19	1
2:B:146:HIS:HE1	2:D:139:ASN:HD22	0.51	1.45	20	1
1:C:20:HIS:O	1:C:24:TYR:CE2	0.51	2.64	1	2
1:A:32:MET:CE	3:A:142:HEC:CBC	0.51	2.88	5	4
1:A:2:LEU:HD13	1:A:131:SER:OG	0.51	2.05	5	1
1:A:31:ARG:CZ	1:A:104:CYS:SG	0.51	2.98	7	1
2:B:145:TYR:CE1	2:B:146:HIS:OXT	0.51	2.63	10	1
2:D:63:HIS:CE1	3:D:147:HEC:C3D	0.51	2.93	19	1
2:D:80:ASN:OD1	2:D:83:GLY:N	0.51	2.42	11	6
1:A:48:LEU:N	1:A:48:LEU:HD22	0.51	2.19	2	3
1:C:48:LEU:N	1:C:48:LEU:HD22	0.51	2.19	2	3
2:D:144:LYS:O	2:D:146:HIS:ND1	0.51	2.44	11	5
1:A:27:GLU:OE1	1:A:112:HIS:CE1	0.51	2.64	3	1
1:A:57:GLY:O	1:A:61:LYS:NZ	0.51	2.41	3	1
1:A:106:LEU:N	1:A:106:LEU:HD12	0.51	2.19	3	1
2:B:21:ASP:OD1	2:B:22:GLU:N	0.51	2.42	3	2
1:C:57:GLY:O	1:C:61:LYS:NZ	0.51	2.41	3	2
1:C:106:LEU:N	1:C:106:LEU:HD12	0.51	2.19	3	4
1:A:48:LEU:HD12	1:A:48:LEU:N	0.51	2.20	8	2
2:B:63:HIS:CE1	3:B:147:HEC:O2A	0.51	2.63	5	1
1:A:10:VAL:HG21	1:A:128:PHE:CD2	0.51	2.40	10	3
2:D:99:ASP:O	2:D:102:ASN:ND2	0.51	2.43	16	2
1:A:17:VAL:O	1:A:20:HIS:N	0.51	2.40	16	3
2:B:102:ASN:OD1	3:B:147:HEC:HMC1	0.51	2.03	12	1
2:D:36:PRO:O	3:D:147:HEC:CMC	0.51	2.55	12	1
2:D:80:ASN:N	2:D:80:ASN:HD22	0.51	2.02	14	1
1:A:32:MET:O	1:A:34:LEU:N	0.51	2.43	16	2
2:D:142:ALA:O	2:D:146:HIS:N	0.51	2.44	17	1
1:A:34:LEU:HD11	2:B:128:ALA:H	0.51	1.64	18	1
1:A:90:LYS:C	1:A:92:ARG:H	0.51	2.08	3	3
2:B:22:GLU:O	2:B:25:GLY:N	0.51	2.42	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:GLU:OE1	1:C:112:HIS:CE1	0.51	2.64	3	1
1:A:26:ALA:HB1	1:A:55:VAL:O	0.51	2.04	8	2
1:A:117:PHE:HZ	2:B:116:HIS:CE1	0.51	2.18	4	1
1:A:107:VAL:O	1:A:110:ALA:HB3	0.51	2.04	5	5
1:A:61:LYS:O	3:A:142:HEC:HMA3	0.51	2.05	9	3
2:B:48:LEU:N	2:B:48:LEU:CD1	0.51	2.74	16	4
1:A:87:HIS:NE2	1:A:136:LEU:O	0.51	2.42	10	1
1:A:96:VAL:HG11	2:D:99:ASP:CB	0.51	2.34	11	1
1:C:105:LEU:HD11	1:C:125:LEU:HD13	0.51	1.82	13	1
1:A:92:ARG:C	2:D:40:ARG:HH12	0.51	2.07	14	1
2:B:146:HIS:HB3	2:D:132:LYS:HG3	0.51	1.81	19	1
1:C:86:LEU:HD21	3:C:142:HEC:CBD	0.51	2.35	13	4
2:B:128:ALA:O	2:B:132:LYS:NZ	0.51	2.43	3	1
1:A:3:SER:N	1:A:6:ASP:OD2	0.51	2.39	20	2
2:B:23:VAL:O	2:B:27:ALA:N	0.51	2.42	5	1
1:C:93:VAL:CG1	1:C:94:ASP:N	0.51	2.73	18	2
2:D:39:GLN:O	3:D:147:HEC:C4D	0.51	2.58	12	1
2:D:42:PHE:CZ	2:D:45:PHE:CE2	0.51	2.98	16	1
2:B:40:ARG:CG	1:C:92:ARG:HD3	0.51	2.36	17	1
1:A:72:HIS:C	1:A:74:ASP:H	0.51	2.09	11	20
2:B:3:LEU:HD13	2:B:8:LYS:HB2	0.51	1.82	1	4
1:C:45:HIS:O	1:C:45:HIS:CG	0.51	2.61	15	2
1:C:83:LEU:O	1:C:87:HIS:ND1	0.51	2.42	14	3
1:A:103:HIS:CD2	2:B:108:ASN:OD1	0.51	2.63	5	2
1:C:117:PHE:O	1:C:117:PHE:CD2	0.51	2.64	7	2
1:A:76:MET:N	1:A:77:PRO:HD2	0.51	2.20	13	4
2:B:99:ASP:O	2:B:102:ASN:ND2	0.51	2.43	16	2
1:A:2:LEU:O	1:A:3:SER:CB	0.51	2.59	10	1
1:A:86:LEU:HD11	3:A:142:HEC:CGD	0.51	2.36	12	1
2:B:91:LEU:HD23	2:B:92:HIS:N	0.51	2.20	12	1
2:D:21:ASP:OD1	2:D:65:LYS:NZ	0.51	2.43	12	1
2:B:146:HIS:CD2	2:D:2:HIS:CE1	0.51	2.78	15	1
3:B:147:HEC:HBC2	2:D:31:LEU:CD2	0.51	2.36	15	1
1:A:36:PHE:CZ	1:A:100:LEU:HD22	0.51	2.41	16	1
2:B:111:VAL:CG2	2:B:130:TYR:CD1	0.51	2.93	18	1
2:B:63:HIS:CE1	3:B:147:HEC:C3D	0.51	2.93	19	1
2:D:3:LEU:HD13	2:D:8:LYS:HB2	0.51	1.83	17	4
2:D:114:LEU:O	2:D:118:PHE:N	0.51	2.44	7	5
2:D:14:LEU:O	2:D:16:GLY:N	0.51	2.44	19	6
1:C:31:ARG:NH2	2:D:127:GLN:CB	0.51	2.73	4	1
2:B:145:TYR:CD1	2:B:145:TYR:C	0.51	2.83	19	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:108:ASN:ND2	2:D:108:ASN:O	0.51	2.44	8	1
2:D:100:PRO:O	2:D:102:ASN:ND2	0.51	2.43	9	1
3:B:147:HEC:C1B	2:D:67:VAL:HG22	0.51	2.35	15	1
3:B:147:HEC:HMD3	2:D:42:PHE:CZ	0.51	2.40	15	1
2:B:103:PHE:O	3:B:147:HEC:HBB1	0.51	2.05	16	1
2:B:145:TYR:CD1	2:B:146:HIS:N	0.51	2.77	16	2
2:D:14:LEU:HD12	2:D:14:LEU:N	0.51	2.20	20	1
1:A:45:HIS:O	1:A:45:HIS:CG	0.51	2.61	15	3
1:A:83:LEU:O	1:A:86:LEU:N	0.51	2.42	4	2
1:A:109:LEU:O	1:A:113:LEU:O	0.51	2.29	14	8
1:A:113:LEU:O	1:A:113:LEU:CD1	0.51	2.58	2	3
1:C:98:PHE:CE1	1:C:102:SER:OG	0.51	2.63	7	1
1:C:103:HIS:N	1:C:103:HIS:ND1	0.51	2.58	7	1
2:B:42:PHE:CE1	2:B:45:PHE:CD2	0.51	2.98	8	1
2:B:80:ASN:N	2:B:80:ASN:HD22	0.51	2.03	14	1
2:B:15:TRP:NE1	2:B:72:SER:OG	0.51	2.43	15	1
2:D:139:ASN:OD1	2:D:139:ASN:N	0.51	2.42	17	2
2:D:3:LEU:HD21	2:D:133:VAL:HG22	0.51	1.81	15	4
2:B:38:THR:O	2:B:40:ARG:N	0.51	2.44	2	2
2:B:99:ASP:OD1	1:C:94:ASP:CG	0.51	2.49	2	1
2:D:102:ASN:O	3:D:147:HEC:HMC2	0.51	2.06	2	1
1:A:103:HIS:ND1	1:A:103:HIS:N	0.51	2.58	7	1
1:A:117:PHE:O	1:A:117:PHE:CD2	0.51	2.64	7	2
1:A:107:VAL:CG1	2:B:127:GLN:HE22	0.51	2.19	8	1
1:A:103:HIS:HB3	2:B:108:ASN:HD21	0.51	1.65	10	1
1:C:46:PHE:CG	1:C:46:PHE:O	0.51	2.64	11	1
2:D:103:PHE:O	3:D:147:HEC:HBB1	0.51	2.05	16	1
1:C:61:LYS:HB3	3:C:142:HEC:C4A	0.51	2.35	19	1
2:D:17:LYS:O	2:D:118:PHE:CZ	0.51	2.65	9	4
1:C:113:LEU:O	1:C:113:LEU:CD1	0.51	2.59	2	3
2:D:38:THR:O	2:D:40:ARG:N	0.51	2.44	2	2
1:A:34:LEU:O	1:A:36:PHE:N	0.51	2.44	6	1
2:B:80:ASN:OD1	2:B:80:ASN:N	0.51	2.44	10	3
1:A:38:THR:HA	2:D:97:HIS:ND1	0.51	2.21	7	1
1:A:105:LEU:HD11	1:A:125:LEU:HD13	0.51	1.82	13	1
1:C:36:PHE:CZ	1:C:100:LEU:HD22	0.51	2.41	16	1
2:B:107:GLY:O	2:B:109:VAL:N	0.51	2.44	19	1
2:B:102:ASN:O	3:B:147:HEC:HMC2	0.50	2.06	2	1
1:C:95:PRO:O	1:C:98:PHE:N	0.50	2.41	4	8
1:C:117:PHE:HZ	2:D:116:HIS:CE1	0.50	2.18	4	1
2:D:145:TYR:CD1	2:D:145:TYR:C	0.50	2.83	19	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:48:LEU:HD12	1:C:48:LEU:N	0.50	2.20	8	1
1:A:66:LEU:HD12	1:A:66:LEU:C	0.50	2.25	17	2
1:A:124:SER:O	1:A:128:PHE:N	0.50	2.44	17	2
1:C:99:LYS:O	1:C:103:HIS:ND1	0.50	2.44	15	1
2:B:32:LEU:O	2:B:36:PRO:N	0.50	2.43	1	4
1:C:100:LEU:O	1:C:104:CYS:SG	0.50	2.70	10	15
1:C:116:GLU:O	1:C:117:PHE:CB	0.50	2.60	5	5
1:A:101:LEU:HD22	3:A:142:HEC:CAB	0.50	2.36	9	2
2:B:144:LYS:O	2:B:146:HIS:ND1	0.50	2.44	11	5
1:C:109:LEU:O	1:C:113:LEU:O	0.50	2.29	14	8
2:B:96:LEU:N	2:B:96:LEU:CD2	0.50	2.74	3	2
1:A:87:HIS:O	1:A:93:VAL:N	0.50	2.44	9	1
2:B:117:HIS:N	2:B:117:HIS:HD1	0.50	2.03	12	1
2:B:14:LEU:N	2:B:14:LEU:HD12	0.50	2.20	20	1
1:A:20:HIS:O	1:A:24:TYR:CE2	0.50	2.63	1	2
1:A:100:LEU:N	1:A:100:LEU:CD1	0.50	2.75	1	2
2:B:84:THR:HG23	2:B:85:PHE:N	0.50	2.22	8	13
2:D:63:HIS:CE1	3:D:147:HEC:O2A	0.50	2.63	5	1
1:C:86:LEU:HG	3:C:142:HEC:HBD1	0.50	1.82	7	1
1:C:66:LEU:HD12	1:C:66:LEU:C	0.50	2.25	17	2
1:C:2:LEU:O	1:C:3:SER:CB	0.50	2.59	10	1
1:C:32:MET:O	1:C:34:LEU:N	0.50	2.43	16	2
1:A:119:PRO:HA	2:B:33:VAL:HG11	0.50	1.82	17	1
2:B:142:ALA:O	2:B:146:HIS:N	0.50	2.44	17	1
1:A:72:HIS:O	1:A:73:VAL:CG1	0.50	2.60	5	20
1:C:72:HIS:O	1:C:73:VAL:CG1	0.50	2.60	5	20
1:C:72:HIS:C	1:C:74:ASP:H	0.50	2.09	1	20
2:D:115:ALA:O	2:D:119:GLY:CA	0.50	2.60	10	16
1:C:76:MET:CE	1:C:131:SER:OG	0.50	2.60	4	5
2:D:96:LEU:C	2:D:97:HIS:ND1	0.50	2.65	12	3
1:A:24:TYR:CD1	1:A:24:TYR:N	0.50	2.78	20	5
2:D:50:THR:HG1	2:D:52:ASP:CG	0.50	2.09	5	1
2:D:71:PHE:CE2	3:D:147:HEC:HMB1	0.50	2.42	5	2
1:C:86:LEU:CD1	1:C:86:LEU:C	0.50	2.79	7	1
1:C:107:VAL:CG1	2:D:127:GLN:HE22	0.50	2.19	8	1
2:B:30:ARG:O	2:B:33:VAL:N	0.50	2.43	9	2
1:A:85:ASP:N	1:A:85:ASP:OD1	0.50	2.44	11	1
1:A:86:LEU:CD2	3:A:142:HEC:CBD	0.50	2.89	12	1
2:D:28:LEU:N	2:D:28:LEU:HD22	0.50	2.21	13	2
1:C:34:LEU:HD11	2:D:128:ALA:H	0.50	1.65	18	1
2:D:107:GLY:O	2:D:109:VAL:N	0.50	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:O	1:A:104:CYS:SG	0.50	2.68	6	13
1:A:21:ALA:C	1:A:23:GLU:N	0.50	2.65	5	16
2:D:96:LEU:N	2:D:96:LEU:CD2	0.50	2.74	3	2
2:B:71:PHE:CE2	3:B:147:HEC:HMB1	0.50	2.42	5	2
1:C:34:LEU:O	1:C:36:PHE:N	0.50	2.44	6	1
1:A:47:ASP:C	1:A:49:SER:H	0.50	2.10	14	9
2:D:63:HIS:O	2:D:63:HIS:ND1	0.50	2.43	14	3
2:B:21:ASP:OD1	2:B:65:LYS:NZ	0.50	2.43	12	1
1:A:126:ASP:OD2	2:B:35:TYR:OH	0.50	2.25	17	1
1:C:32:MET:HE1	3:C:142:HEC:HBC2	0.50	1.82	19	1
2:B:127:GLN:CD	2:B:127:GLN:H	0.50	2.09	20	1
1:A:128:PHE:O	1:A:128:PHE:CD1	0.50	2.65	10	13
1:A:53:ALA:O	1:A:56:LYS:N	0.50	2.42	13	3
1:C:58:HIS:ND1	1:C:58:HIS:O	0.50	2.45	18	3
2:B:33:VAL:CG1	2:B:34:VAL:N	0.50	2.75	3	2
2:B:97:HIS:O	1:C:38:THR:HG22	0.50	2.07	3	1
1:C:99:LYS:CD	1:C:99:LYS:N	0.50	2.75	7	1
1:A:46:PHE:CG	1:A:46:PHE:O	0.50	2.64	11	2
1:C:1:VAL:CG1	1:C:131:SER:OG	0.50	2.60	12	1
1:C:33:PHE:HE1	3:C:142:HEC:ND	0.50	2.04	12	1
1:C:53:ALA:O	1:C:56:LYS:N	0.50	2.42	13	2
1:C:93:VAL:CG2	1:C:94:ASP:N	0.50	2.75	13	1
2:D:41:PHE:HE1	3:D:147:HEC:NB	0.50	2.02	15	1
1:A:56:LYS:H	1:A:56:LYS:CD	0.50	2.20	5	2
2:B:4:THR:O	2:B:6:GLU:N	0.50	2.45	14	6
1:C:52:SER:C	1:C:54:GLN:N	0.50	2.65	1	2
2:D:4:THR:O	2:D:6:GLU:N	0.50	2.45	14	7
2:B:14:LEU:O	2:B:16:GLY:N	0.50	2.45	2	6
2:B:96:LEU:C	2:B:97:HIS:ND1	0.50	2.65	12	3
2:B:108:ASN:O	2:B:108:ASN:ND2	0.50	2.44	8	2
2:B:99:ASP:O	2:B:100:PRO:O	0.50	2.30	17	5
1:C:87:HIS:O	1:C:93:VAL:N	0.50	2.44	9	1
1:C:119:PRO:HB3	2:D:51:PRO:HB3	0.50	1.83	11	1
1:A:1:VAL:CG1	1:A:131:SER:OG	0.50	2.60	12	1
1:A:93:VAL:CG2	1:A:94:ASP:N	0.50	2.75	13	1
1:A:99:LYS:O	1:A:103:HIS:ND1	0.50	2.44	15	1
1:A:18:GLY:C	1:A:20:HIS:H	0.50	2.10	16	18
1:A:116:GLU:O	1:A:117:PHE:CB	0.50	2.60	5	5
1:A:118:THR:OG1	1:A:121:VAL:HB	0.50	2.07	20	6
2:B:8:LYS:O	2:B:12:THR:OG1	0.50	2.29	8	14
2:B:114:LEU:O	2:B:118:PHE:N	0.50	2.44	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:2:LEU:CD1	1:C:2:LEU:N	0.50	2.75	2	2
1:A:58:HIS:ND1	1:A:58:HIS:O	0.50	2.45	18	3
2:B:134:VAL:O	2:B:137:VAL:N	0.50	2.45	9	7
2:D:96:LEU:N	2:D:96:LEU:HD22	0.50	2.22	16	2
2:B:97:HIS:CB	1:C:38:THR:HA	0.50	2.34	4	1
1:A:119:PRO:HB3	2:B:51:PRO:HB3	0.50	1.83	11	1
2:B:143:HIS:O	2:B:146:HIS:CD2	0.50	2.65	18	1
1:C:11:LYS:N	1:C:11:LYS:CD	0.50	2.75	15	3
1:C:18:GLY:C	1:C:20:HIS:H	0.50	2.10	16	17
1:C:3:SER:N	1:C:6:ASP:OD2	0.50	2.40	20	2
2:B:94:ASP:O	1:C:41:THR:HG21	0.50	2.07	6	1
1:A:35:SER:OG	1:A:36:PHE:CD2	0.50	2.62	7	1
1:A:96:VAL:CG1	2:D:99:ASP:CG	0.50	2.53	11	1
2:B:28:LEU:N	2:B:28:LEU:HD22	0.50	2.21	13	2
2:D:106:LEU:CB	3:D:147:HEC:HAB	0.50	2.37	13	1
2:D:63:HIS:HE1	3:D:147:HEC:C2A	0.50	2.19	16	1
2:D:67:VAL:HG13	3:D:147:HEC:C3B	0.50	2.34	18	1
1:C:17:VAL:CG1	1:C:21:ALA:HB2	0.49	2.37	1	1
2:B:115:ALA:O	2:B:119:GLY:CA	0.49	2.60	6	15
2:D:84:THR:HG23	2:D:85:PHE:N	0.49	2.22	8	13
1:A:98:PHE:CD1	1:A:98:PHE:C	0.49	2.85	6	3
1:C:47:ASP:C	1:C:49:SER:H	0.49	2.10	14	8
2:D:48:LEU:N	2:D:48:LEU:CD1	0.49	2.74	16	4
2:D:42:PHE:C	3:D:147:HEC:C3A	0.49	2.81	12	1
2:B:106:LEU:CB	3:B:147:HEC:HAB	0.49	2.37	13	1
2:B:106:LEU:CD1	2:B:106:LEU:C	0.49	2.81	18	1
1:A:17:VAL:CG1	1:A:21:ALA:HB2	0.49	2.37	1	1
2:B:97:HIS:CD2	1:C:38:THR:CG2	0.49	2.96	1	1
2:B:19:ASN:O	2:B:22:GLU:N	0.49	2.42	9	7
2:D:120:LYS:N	2:D:120:LYS:CD	0.49	2.75	11	1
2:D:131:GLN:CD	2:D:131:GLN:H	0.49	2.10	15	2
2:D:143:HIS:O	2:D:146:HIS:CD2	0.49	2.65	18	1
1:C:118:THR:OG1	1:C:121:VAL:HB	0.49	2.07	20	6
1:C:128:PHE:O	1:C:128:PHE:CD1	0.49	2.65	10	13
1:C:21:ALA:C	1:C:23:GLU:N	0.49	2.65	18	16
1:A:76:MET:CE	1:A:131:SER:OG	0.49	2.61	12	5
2:B:131:GLN:O	2:B:135:ALA:HB2	0.49	2.07	15	4
2:B:37:TRP:CD1	2:B:37:TRP:N	0.49	2.79	20	2
2:B:40:ARG:HG3	1:C:92:ARG:CZ	0.49	2.37	15	1
2:D:63:HIS:ND1	2:D:63:HIS:O	0.49	2.45	18	2
1:A:49:SER:C	1:A:50:HIS:CG	0.49	2.85	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:101:LEU:HD22	3:C:142:HEC:CAB	0.49	2.36	9	2
1:A:99:LYS:N	1:A:99:LYS:CD	0.49	2.75	7	1
1:C:101:LEU:HD11	3:C:142:HEC:CHC	0.49	2.32	7	1
1:C:33:PHE:HE1	3:C:142:HEC:C4D	0.49	2.20	12	1
2:D:39:GLN:HG2	3:D:147:HEC:C4B	0.49	2.32	12	1
2:B:95:LYS:CA	2:B:97:HIS:NE2	0.49	2.75	15	1
1:C:108:THR:OG1	1:C:109:LEU:N	0.49	2.45	20	1
1:A:118:THR:C	1:A:120:ALA:N	0.49	2.64	18	18
1:C:118:THR:C	1:C:120:ALA:N	0.49	2.64	18	12
1:A:106:LEU:HD12	1:A:106:LEU:N	0.49	2.21	17	3
2:B:131:GLN:CD	2:B:131:GLN:H	0.49	2.10	15	2
1:A:92:ARG:CZ	2:D:40:ARG:HD2	0.49	2.38	18	1
1:A:93:VAL:CG1	1:A:94:ASP:H	0.49	2.21	18	1
2:D:8:LYS:O	2:D:12:THR:OG1	0.49	2.30	16	15
1:A:99:LYS:NZ	1:A:99:LYS:CB	0.49	2.76	16	2
2:D:131:GLN:O	2:D:135:ALA:HB2	0.49	2.07	15	4
1:C:1:VAL:O	1:C:2:LEU:CB	0.49	2.60	10	2
2:B:63:HIS:O	2:B:63:HIS:ND1	0.49	2.43	10	5
1:C:27:GLU:OE1	1:C:112:HIS:CD2	0.49	2.66	10	1
1:C:33:PHE:CE1	3:C:142:HEC:ND	0.49	2.81	12	1
1:A:46:PHE:O	1:A:48:LEU:CD2	0.49	2.61	14	1
1:A:115:ALA:C	1:A:117:PHE:N	0.49	2.64	15	2
1:C:50:HIS:CD2	1:C:50:HIS:N	0.49	2.81	19	2
1:A:50:HIS:N	1:A:50:HIS:CD2	0.49	2.81	19	1
1:C:49:SER:C	1:C:50:HIS:CG	0.49	2.85	19	1
1:A:129:LEU:C	1:A:129:LEU:CD1	0.49	2.80	20	1
2:D:106:LEU:HD21	3:D:147:HEC:C3B	0.49	2.37	2	1
2:D:23:VAL:O	2:D:27:ALA:N	0.49	2.41	5	1
1:A:106:LEU:N	1:A:106:LEU:CD1	0.49	2.76	17	3
1:C:10:VAL:HG21	1:C:128:PHE:CG	0.49	2.43	9	2
1:C:119:PRO:HA	2:D:33:VAL:HG11	0.49	1.82	17	1
2:B:43:GLU:OE2	1:C:92:ARG:NH1	0.49	2.46	20	1
2:D:127:GLN:CD	2:D:127:GLN:H	0.49	2.09	20	1
2:B:17:LYS:O	2:B:118:PHE:CZ	0.49	2.64	9	4
1:A:32:MET:CE	3:A:142:HEC:HBC2	0.49	2.38	2	3
2:B:106:LEU:HD21	3:B:147:HEC:C3B	0.49	2.37	2	1
2:D:134:VAL:O	2:D:137:VAL:N	0.49	2.45	9	7
2:D:95:LYS:N	2:D:95:LYS:CD	0.49	2.76	6	2
1:C:61:LYS:O	3:C:142:HEC:CMA	0.49	2.61	9	4
2:B:120:LYS:CD	2:B:120:LYS:N	0.49	2.75	11	1
1:C:46:PHE:O	1:C:48:LEU:CD2	0.49	2.61	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:96:LEU:HD22	2:B:96:LEU:N	0.49	2.22	16	1
1:A:2:LEU:CD1	1:A:2:LEU:N	0.49	2.75	2	2
1:A:86:LEU:O	1:A:90:LYS:O	0.49	2.31	8	7
2:B:42:PHE:C	2:B:44:SER:N	0.49	2.66	7	2
1:C:98:PHE:CD1	1:C:98:PHE:C	0.49	2.85	19	3
1:C:106:LEU:N	1:C:106:LEU:CD1	0.49	2.75	17	2
1:A:10:VAL:HG21	1:A:128:PHE:CG	0.49	2.43	9	1
2:D:99:ASP:O	2:D:100:PRO:O	0.49	2.31	15	5
1:C:105:LEU:C	1:C:105:LEU:CD1	0.49	2.80	13	2
1:A:116:GLU:C	1:A:117:PHE:CG	0.49	2.86	14	3
2:D:95:LYS:CA	2:D:97:HIS:NE2	0.49	2.76	15	1
2:D:94:ASP:OD1	2:D:94:ASP:N	0.49	2.46	3	3
1:C:36:PHE:CD1	1:C:100:LEU:HD13	0.49	2.43	5	1
2:D:93:CYS:SG	2:D:94:ASP:OD2	0.49	2.71	10	1
1:A:93:VAL:O	2:D:40:ARG:CZ	0.49	2.61	14	1
1:A:116:GLU:C	1:A:117:PHE:CD2	0.49	2.87	14	2
2:D:95:LYS:C	2:D:97:HIS:NE2	0.49	2.66	15	1
1:A:92:ARG:NH1	2:D:40:ARG:CB	0.49	2.69	18	1
1:A:108:THR:OG1	1:A:109:LEU:N	0.49	2.45	20	1
1:C:86:LEU:O	1:C:90:LYS:O	0.48	2.31	8	7
1:A:61:LYS:HB3	3:A:142:HEC:HMA3	0.48	1.84	2	1
1:C:118:THR:OG1	1:C:121:VAL:N	0.48	2.43	12	4
1:A:95:PRO:C	1:A:97:ASN:H	0.48	2.12	13	4
1:A:1:VAL:O	1:A:2:LEU:CB	0.48	2.60	10	2
2:B:36:PRO:O	2:B:38:THR:N	0.48	2.46	15	2
1:A:27:GLU:OE1	1:A:112:HIS:CD2	0.48	2.66	10	1
1:A:2:LEU:CD1	1:A:128:PHE:CD2	0.48	2.96	16	2
1:C:115:ALA:C	1:C:117:PHE:N	0.48	2.63	15	2
2:B:95:LYS:C	2:B:97:HIS:NE2	0.48	2.67	15	1
1:A:113:LEU:O	1:A:113:LEU:CG	0.48	2.61	2	4
1:C:5:ALA:O	1:C:6:ASP:C	0.48	2.51	10	19
1:C:56:LYS:CD	1:C:56:LYS:H	0.48	2.21	1	2
2:B:96:LEU:N	2:B:96:LEU:HD22	0.48	2.22	3	1
1:C:95:PRO:C	1:C:97:ASN:H	0.48	2.11	13	4
2:B:146:HIS:OXT	2:B:146:HIS:ND1	0.48	2.46	4	2
2:B:144:LYS:C	2:B:146:HIS:N	0.48	2.67	19	7
2:B:95:LYS:CD	2:B:95:LYS:N	0.48	2.76	6	2
1:A:94:ASP:OD2	2:D:97:HIS:CE1	0.48	2.67	10	1
1:C:48:LEU:HD12	3:C:142:HEC:HHA	0.48	1.82	12	1
1:C:124:SER:O	1:C:128:PHE:N	0.48	2.44	17	2
1:C:116:GLU:C	1:C:117:PHE:CG	0.48	2.86	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:63:HIS:HE1	3:B:147:HEC:C2A	0.48	2.19	16	1
2:B:40:ARG:HB3	1:C:92:ARG:HD3	0.48	1.84	17	1
2:B:146:HIS:HE2	2:D:136:GLY:N	0.48	2.05	17	1
2:D:28:LEU:N	2:D:28:LEU:CD1	0.48	2.76	18	2
2:D:66:LYS:CB	3:D:147:HEC:HBA2	0.48	2.38	17	1
1:A:31:ARG:O	1:A:34:LEU:CD2	0.48	2.61	1	1
2:D:17:LYS:O	2:D:118:PHE:CE2	0.48	2.67	9	2
2:D:52:ASP:OD1	2:D:52:ASP:N	0.48	2.46	9	1
2:D:87:THR:O	2:D:91:LEU:N	0.48	2.47	12	3
1:C:85:ASP:N	1:C:85:ASP:OD1	0.48	2.44	11	2
1:A:129:LEU:HD21	3:A:142:HEC:HBB1	0.48	1.85	13	1
1:A:31:ARG:HH21	2:B:127:GLN:CB	0.48	2.18	15	1
2:B:42:PHE:CZ	2:B:45:PHE:CZ	0.48	3.01	16	1
1:C:40:LYS:O	1:C:41:THR:C	0.48	2.52	18	2
1:A:11:LYS:N	1:A:11:LYS:CD	0.48	2.75	1	3
1:C:113:LEU:O	1:C:113:LEU:CG	0.48	2.61	20	4
2:D:19:ASN:C	2:D:21:ASP:N	0.48	2.66	16	13
1:C:21:ALA:HB1	1:C:63:ALA:HB1	0.48	1.85	2	2
1:A:96:VAL:HG11	2:D:99:ASP:OD1	0.48	2.07	6	1
1:C:32:MET:SD	1:C:32:MET:C	0.48	2.92	6	2
2:B:93:CYS:SG	2:B:94:ASP:OD2	0.48	2.71	10	1
1:C:2:LEU:CD1	1:C:128:PHE:CD2	0.48	2.96	16	2
2:B:40:ARG:CG	1:C:92:ARG:CZ	0.48	2.91	15	1
2:D:42:PHE:CZ	2:D:45:PHE:CZ	0.48	3.01	16	1
1:C:101:LEU:HD23	1:C:101:LEU:C	0.48	2.29	19	1
2:B:19:ASN:C	2:B:21:ASP:N	0.48	2.67	4	13
2:D:146:HIS:ND1	2:D:146:HIS:N	0.48	2.61	1	2
1:A:91:LEU:C	1:A:93:VAL:N	0.48	2.67	20	8
2:D:42:PHE:C	2:D:44:SER:N	0.48	2.66	7	2
2:D:33:VAL:CG1	2:D:34:VAL:N	0.48	2.77	11	2
2:B:72:SER:O	2:B:76:ALA:HB3	0.48	2.09	4	1
2:B:119:GLY:O	2:B:122:PHE:N	0.48	2.47	19	2
2:B:8:LYS:C	2:B:8:LYS:CD	0.48	2.81	9	1
1:A:85:ASP:OD1	1:A:85:ASP:N	0.48	2.47	17	2
2:B:66:LYS:CB	3:B:147:HEC:HBA2	0.48	2.38	17	1
2:B:135:ALA:HB3	2:D:146:HIS:CE1	0.48	2.43	17	1
2:B:40:ARG:HD2	1:C:92:ARG:CZ	0.48	2.38	18	1
1:A:101:LEU:C	1:A:101:LEU:HD23	0.48	2.29	19	1
1:C:131:SER:O	1:C:135:VAL:HG23	0.48	2.09	19	2
1:A:52:SER:C	1:A:54:GLN:N	0.48	2.65	1	2
1:C:31:ARG:O	1:C:34:LEU:CD2	0.48	2.61	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:32:MET:CE	3:C:142:HEC:HBC2	0.48	2.38	2	3
1:C:99:LYS:CB	1:C:99:LYS:NZ	0.48	2.76	16	2
1:A:95:PRO:C	1:A:97:ASN:N	0.48	2.66	10	8
1:A:47:ASP:C	1:A:49:SER:N	0.48	2.67	20	12
2:B:17:LYS:O	2:B:118:PHE:CE2	0.48	2.67	9	2
1:C:109:LEU:O	1:C:114:PRO:N	0.48	2.47	6	3
2:D:36:PRO:O	2:D:38:THR:N	0.48	2.46	15	2
1:C:32:MET:HE1	3:C:142:HEC:C3B	0.48	2.39	12	1
1:C:32:MET:HE1	3:C:142:HEC:CAB	0.48	2.30	12	1
1:C:126:ASP:OD2	2:D:35:TYR:OH	0.48	2.25	17	1
2:B:40:ARG:NE	1:C:92:ARG:HB3	0.48	2.23	18	1
2:B:40:ARG:NH2	1:C:92:ARG:HB2	0.48	2.22	18	1
2:D:106:LEU:CD1	2:D:106:LEU:C	0.48	2.81	18	1
1:A:38:THR:CG2	2:D:97:HIS:CD2	0.48	2.97	1	1
1:A:46:PHE:CD1	1:A:46:PHE:C	0.48	2.85	9	4
1:C:115:ALA:O	1:C:121:VAL:CG2	0.48	2.60	1	1
1:C:95:PRO:C	1:C:97:ASN:N	0.48	2.67	10	10
1:C:27:GLU:CD	1:C:112:HIS:CE1	0.48	2.87	3	1
1:A:36:PHE:CD1	1:A:100:LEU:HD13	0.48	2.43	5	1
2:B:45:PHE:C	2:B:47:ASP:N	0.48	2.66	5	1
2:B:50:THR:HG1	2:B:52:ASP:CG	0.48	2.12	5	2
2:D:37:TRP:NE1	2:D:38:THR:HG23	0.48	2.24	5	4
2:D:88:LEU:N	2:D:88:LEU:HD12	0.48	2.24	14	3
2:B:63:HIS:HE1	3:B:147:HEC:HHA	0.48	1.64	12	1
2:D:39:GLN:NE2	3:D:147:HEC:NB	0.48	2.61	12	1
1:C:93:VAL:CG2	1:C:94:ASP:H	0.48	2.17	13	1
1:C:129:LEU:HD21	3:C:142:HEC:HBB1	0.48	1.85	13	1
2:B:40:ARG:HH12	1:C:92:ARG:C	0.48	2.12	14	1
2:D:76:ALA:C	2:D:77:HIS:CG	0.48	2.86	14	1
2:B:95:LYS:C	2:B:97:HIS:CD2	0.48	2.87	15	1
3:B:147:HEC:HBA2	2:D:66:LYS:HB3	0.48	1.84	15	1
1:A:131:SER:O	1:A:135:VAL:HG23	0.48	2.09	19	2
2:B:94:ASP:OD1	2:B:94:ASP:N	0.48	2.46	3	3
1:C:47:ASP:C	1:C:49:SER:N	0.48	2.67	9	13
1:C:83:LEU:O	1:C:87:HIS:CE1	0.48	2.67	10	3
1:C:46:PHE:C	1:C:48:LEU:N	0.48	2.67	10	5
1:C:129:LEU:HD12	1:C:129:LEU:O	0.48	2.08	6	1
1:A:61:LYS:O	3:A:142:HEC:CMA	0.48	2.61	9	4
2:B:52:ASP:OD1	2:B:52:ASP:N	0.48	2.46	9	1
2:D:8:LYS:C	2:D:8:LYS:CD	0.48	2.81	9	1
1:A:6:ASP:OD1	1:A:7:LYS:N	0.48	2.47	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:31:LEU:HD21	3:B:147:HEC:HBC2	0.48	1.86	10	1
1:A:92:ARG:NH1	2:D:40:ARG:HA	0.48	2.24	12	1
1:A:35:SER:C	1:A:36:PHE:CD2	0.48	2.87	15	1
2:B:20:VAL:O	2:B:22:GLU:N	0.48	2.47	15	1
2:D:20:VAL:O	2:D:22:GLU:N	0.48	2.47	15	1
1:A:5:ALA:O	1:A:6:ASP:C	0.48	2.51	10	19
1:C:61:LYS:HB3	3:C:142:HEC:HMA3	0.48	1.84	2	1
1:C:52:SER:O	1:C:53:ALA:CB	0.48	2.61	3	7
2:D:71:PHE:CZ	2:D:134:VAL:HG11	0.48	2.44	3	1
1:A:83:LEU:O	1:A:87:HIS:CE1	0.48	2.67	10	3
2:B:103:PHE:CD1	2:B:103:PHE:N	0.48	2.81	5	2
2:D:45:PHE:C	2:D:47:ASP:N	0.48	2.66	5	1
2:D:144:LYS:C	2:D:146:HIS:N	0.48	2.67	16	7
1:C:6:ASP:OD1	1:C:7:LYS:N	0.48	2.47	10	1
2:D:31:LEU:HD21	3:D:147:HEC:HBC2	0.48	1.86	10	1
2:B:76:ALA:C	2:B:77:HIS:CG	0.48	2.86	14	1
1:C:116:GLU:C	1:C:117:PHE:CD2	0.48	2.87	14	2
1:C:3:SER:CB	1:C:4:PRO:CD	0.48	2.92	15	4
1:A:120:ALA:O	1:A:124:SER:CB	0.48	2.62	18	1
1:C:100:LEU:O	1:C:104:CYS:N	0.48	2.46	19	1
1:A:27:GLU:CD	1:A:112:HIS:CE1	0.48	2.87	3	1
2:B:37:TRP:NE1	2:B:38:THR:HG23	0.48	2.24	5	3
2:B:124:PRO:N	2:B:125:PRO:CD	0.48	2.77	15	2
1:C:109:LEU:C	1:C:109:LEU:CD1	0.48	2.81	16	1
1:C:120:ALA:O	1:C:124:SER:CB	0.48	2.62	18	1
2:D:82:LYS:HZ1	2:D:143:HIS:CD2	0.48	2.27	20	1
1:A:124:SER:O	1:A:128:PHE:CB	0.47	2.62	13	9
1:A:127:LYS:C	1:A:127:LYS:CD	0.47	2.82	8	9
2:D:106:LEU:HD13	3:D:147:HEC:HAB	0.47	1.85	3	2
2:D:146:HIS:OXT	2:D:146:HIS:ND1	0.47	2.46	4	2
2:B:96:LEU:HD12	2:B:98:VAL:HG23	0.47	1.87	6	2
2:B:88:LEU:N	2:B:88:LEU:HD12	0.47	2.24	14	3
2:B:117:HIS:C	2:B:118:PHE:CG	0.47	2.87	17	6
2:B:43:GLU:CD	2:B:44:SER:N	0.47	2.67	9	1
2:B:57:ASN:ND2	2:B:59:LYS:N	0.47	2.62	9	1
2:D:43:GLU:CD	2:D:44:SER:N	0.47	2.67	9	1
1:C:35:SER:C	1:C:36:PHE:CD2	0.47	2.87	15	1
2:B:28:LEU:N	2:B:28:LEU:CD1	0.47	2.75	18	2
2:B:44:SER:O	2:B:46:GLY:N	0.47	2.47	3	6
1:C:5:ALA:C	1:C:7:LYS:N	0.47	2.67	12	3
1:C:124:SER:O	1:C:128:PHE:CB	0.47	2.62	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:147:HEC:HHC	3:D:147:HEC:HBB2	0.47	1.87	7	3
2:D:38:THR:C	2:D:40:ARG:N	0.47	2.67	15	2
2:D:117:HIS:C	2:D:118:PHE:CG	0.47	2.87	17	5
1:A:93:VAL:CG2	1:A:94:ASP:H	0.47	2.17	13	1
1:A:3:SER:CB	1:A:4:PRO:CD	0.47	2.92	20	4
2:D:37:TRP:CD1	2:D:37:TRP:N	0.47	2.79	20	1
1:C:91:LEU:O	1:C:92:ARG:C	0.47	2.53	12	2
1:C:127:LYS:C	1:C:127:LYS:CD	0.47	2.83	11	11
2:D:63:HIS:NE2	3:D:147:HEC:HHA	0.47	2.24	2	1
1:A:33:PHE:CD1	1:A:33:PHE:C	0.47	2.87	14	4
2:D:97:HIS:CD2	2:D:97:HIS:O	0.47	2.68	5	1
2:D:116:HIS:C	2:D:116:HIS:HD1	0.47	2.13	19	4
1:A:99:LYS:O	1:A:103:HIS:CG	0.47	2.68	7	1
1:C:86:LEU:CG	3:C:142:HEC:CBD	0.47	2.93	7	1
1:A:48:LEU:CD1	1:A:48:LEU:N	0.47	2.70	9	2
1:A:107:VAL:HG11	2:B:127:GLN:OE1	0.47	2.10	8	1
1:A:27:GLU:CD	1:A:112:HIS:NE2	0.47	2.68	10	1
2:B:100:PRO:O	2:B:102:ASN:N	0.47	2.41	10	1
1:C:137:THR:O	1:C:138:SER:CB	0.47	2.63	15	1
1:C:109:LEU:O	1:C:112:HIS:CD2	0.47	2.68	16	1
2:B:139:ASN:OD1	2:D:146:HIS:HD2	0.47	1.92	17	1
1:A:38:THR:HG22	2:D:97:HIS:HB3	0.47	1.84	19	1
1:A:61:LYS:HG3	3:A:142:HEC:HAA2	0.47	1.86	19	1
1:C:61:LYS:HG3	3:C:142:HEC:HAA2	0.47	1.85	19	1
2:D:103:PHE:CD1	2:D:103:PHE:N	0.47	2.81	5	2
1:A:118:THR:OG1	1:A:121:VAL:N	0.47	2.43	2	5
2:B:38:THR:C	2:B:40:ARG:N	0.47	2.67	15	2
1:C:109:LEU:O	1:C:113:LEU:C	0.47	2.53	6	10
1:A:129:LEU:HD12	1:A:129:LEU:O	0.47	2.08	6	1
2:B:123:THR:OG1	2:B:126:VAL:CG2	0.47	2.63	9	5
2:D:102:ASN:ND2	2:D:103:PHE:CD1	0.47	2.83	6	1
1:C:99:LYS:O	1:C:103:HIS:CG	0.47	2.68	7	1
2:B:42:PHE:O	2:B:42:PHE:CD2	0.47	2.68	8	1
2:B:106:LEU:CD2	3:B:147:HEC:CAB	0.47	2.86	10	1
1:A:109:LEU:O	1:A:112:HIS:CD2	0.47	2.68	16	1
1:C:24:TYR:CE2	1:C:112:HIS:CE1	0.47	3.03	16	1
1:C:34:LEU:HD13	2:D:128:ALA:CB	0.47	2.31	18	1
1:A:86:LEU:C	1:A:86:LEU:CD1	0.47	2.82	19	1
2:D:44:SER:O	2:D:46:GLY:N	0.47	2.47	3	6
1:A:52:SER:O	1:A:53:ALA:CB	0.47	2.61	3	7
2:B:41:PHE:C	2:B:43:GLU:N	0.47	2.67	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:91:LEU:C	1:C:93:VAL:N	0.47	2.68	5	7
1:A:109:LEU:O	1:A:113:LEU:C	0.47	2.53	6	10
2:D:72:SER:O	2:D:76:ALA:HB3	0.47	2.09	4	1
2:B:81:LEU:O	2:B:85:PHE:CE1	0.47	2.68	6	1
1:C:27:GLU:CD	1:C:112:HIS:NE2	0.47	2.68	10	1
1:A:41:THR:CB	2:D:97:HIS:NE2	0.47	2.77	12	2
2:D:123:THR:O	2:D:127:GLN:NE2	0.47	2.47	11	1
1:C:32:MET:SD	3:C:142:HEC:HHC	0.47	2.49	12	1
1:A:92:ARG:O	1:A:93:VAL:HG12	0.47	2.10	13	1
2:D:95:LYS:C	2:D:97:HIS:CD2	0.47	2.87	15	1
2:D:7:GLU:N	2:D:7:GLU:CD	0.47	2.68	20	2
2:D:107:GLY:C	2:D:109:VAL:N	0.47	2.68	19	1
1:A:2:LEU:N	1:A:2:LEU:HD12	0.47	2.24	2	3
1:A:49:SER:O	1:A:50:HIS:O	0.47	2.32	5	5
1:C:53:ALA:C	1:C:55:VAL:N	0.47	2.68	2	5
1:C:46:PHE:O	1:C:46:PHE:CG	0.47	2.67	8	2
1:A:108:THR:O	1:A:110:ALA:N	0.47	2.48	5	5
1:A:109:LEU:O	1:A:114:PRO:N	0.47	2.47	6	3
2:B:116:HIS:C	2:B:116:HIS:HD1	0.47	2.13	19	4
1:C:33:PHE:CD1	1:C:33:PHE:C	0.47	2.87	14	4
1:C:122:HIS:CE1	2:D:112:CYS:SG	0.47	3.08	5	1
1:C:2:LEU:HD21	1:C:6:ASP:OD2	0.47	2.09	8	1
2:B:38:THR:HG22	3:B:147:HEC:HBC1	0.47	1.86	9	1
2:D:38:THR:HG22	3:D:147:HEC:HBC1	0.47	1.86	9	1
2:B:41:PHE:CD2	3:B:147:HEC:CMD	0.47	2.98	12	1
2:B:7:GLU:N	2:B:7:GLU:CD	0.47	2.68	20	2
1:A:33:PHE:O	1:A:36:PHE:N	0.47	2.47	1	1
1:C:46:PHE:CD1	1:C:46:PHE:C	0.47	2.87	1	4
1:A:53:ALA:C	1:A:55:VAL:N	0.47	2.68	14	5
2:B:14:LEU:C	2:B:16:GLY:N	0.47	2.68	19	7
2:B:71:PHE:CZ	2:B:134:VAL:HG11	0.47	2.44	3	1
1:A:41:THR:HB	2:D:97:HIS:ND1	0.47	2.24	4	1
1:A:122:HIS:CE1	2:B:112:CYS:SG	0.47	3.08	5	1
1:C:4:PRO:C	1:C:6:ASP:N	0.47	2.66	7	5
1:A:32:MET:SD	1:A:32:MET:C	0.47	2.92	6	2
2:B:76:ALA:O	2:B:77:HIS:CD2	0.47	2.68	6	4
2:B:146:HIS:C	2:D:139:ASN:OD1	0.47	2.53	6	1
2:D:81:LEU:O	2:D:85:PHE:CE1	0.47	2.68	6	1
1:C:107:VAL:HG11	2:D:127:GLN:OE1	0.47	2.09	8	1
2:D:42:PHE:CD2	2:D:42:PHE:O	0.47	2.67	8	1
1:A:89:HIS:O	1:A:90:LYS:O	0.47	2.33	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:57:ASN:ND2	2:D:59:LYS:N	0.47	2.63	9	1
2:B:87:THR:O	2:B:91:LEU:N	0.47	2.40	11	3
2:D:99:ASP:OD1	2:D:99:ASP:N	0.47	2.48	18	2
2:B:20:VAL:HG12	2:B:20:VAL:O	0.47	2.10	11	2
2:B:123:THR:O	2:B:127:GLN:NE2	0.47	2.47	11	1
2:B:117:HIS:N	2:B:117:HIS:ND1	0.47	2.62	12	1
1:A:101:LEU:HD21	3:A:142:HEC:CBB	0.47	2.30	15	2
2:B:3:LEU:HD23	2:B:132:LYS:HZ1	0.47	1.70	15	1
2:D:124:PRO:N	2:D:125:PRO:CD	0.47	2.77	15	2
2:B:97:HIS:CB	1:C:38:THR:HB	0.47	2.39	19	1
2:B:112:CYS:SG	2:B:113:VAL:N	0.47	2.87	20	1
2:B:142:ALA:O	2:B:144:LYS:N	0.47	2.48	20	1
2:B:146:HIS:ND1	2:B:146:HIS:N	0.47	2.61	1	2
1:C:33:PHE:O	1:C:36:PHE:N	0.47	2.47	1	2
1:A:21:ALA:HB1	1:A:63:ALA:HB1	0.47	1.85	2	2
2:D:145:TYR:O	2:D:145:TYR:CG	0.47	2.64	5	2
2:B:102:ASN:ND2	2:B:103:PHE:CD1	0.47	2.83	6	1
1:C:129:LEU:C	1:C:129:LEU:CD1	0.47	2.79	20	3
1:C:83:LEU:C	1:C:83:LEU:CD1	0.47	2.79	7	1
1:A:2:LEU:HD21	1:A:6:ASP:OD2	0.47	2.10	8	1
2:D:36:PRO:C	3:D:147:HEC:CHC	0.47	2.83	15	1
2:D:41:PHE:CE1	3:D:147:HEC:NB	0.47	2.67	15	1
2:D:142:ALA:O	2:D:144:LYS:N	0.47	2.48	20	1
2:D:4:THR:O	2:D:7:GLU:N	0.47	2.46	16	3
2:D:123:THR:OG1	2:D:126:VAL:CG2	0.47	2.63	9	6
2:D:21:ASP:C	2:D:65:LYS:HZ3	0.47	2.13	10	1
1:C:92:ARG:O	1:C:93:VAL:HG12	0.47	2.10	13	1
2:D:3:LEU:HD23	2:D:132:LYS:HZ1	0.47	1.67	15	1
2:B:91:LEU:O	2:B:95:LYS:CB	0.47	2.63	9	7
1:C:97:ASN:O	1:C:100:LEU:N	0.47	2.41	1	3
1:A:35:SER:C	1:A:36:PHE:CD1	0.47	2.88	13	4
1:C:35:SER:C	1:C:36:PHE:CD1	0.47	2.89	20	4
1:A:37:PRO:C	1:A:39:THR:N	0.47	2.68	10	10
1:C:31:ARG:NH2	2:D:127:GLN:HB3	0.47	2.25	4	1
1:A:4:PRO:C	1:A:6:ASP:N	0.47	2.68	5	5
2:B:97:HIS:CD2	2:B:97:HIS:O	0.47	2.68	5	1
1:C:47:ASP:OD1	1:C:47:ASP:N	0.47	2.46	6	1
1:A:122:HIS:CD2	1:A:122:HIS:H	0.47	2.28	8	1
1:A:41:THR:OG1	2:D:97:HIS:CE1	0.47	2.67	12	1
2:D:117:HIS:N	2:D:117:HIS:ND1	0.47	2.61	12	1
2:D:13:ALA:C	2:D:15:TRP:N	0.47	2.68	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:31:ARG:HH21	2:D:127:GLN:CB	0.47	2.18	15	1
1:C:20:HIS:CB	1:C:24:TYR:CZ	0.47	2.98	16	1
2:B:40:ARG:CB	1:C:92:ARG:HD3	0.47	2.40	17	1
2:B:142:ALA:C	2:B:144:LYS:N	0.47	2.69	20	1
2:B:58:PRO:O	2:B:62:ALA:N	0.46	2.41	2	1
1:A:90:LYS:C	1:A:92:ARG:N	0.46	2.68	16	4
1:C:90:LYS:C	1:C:92:ARG:N	0.46	2.68	16	4
1:A:31:ARG:NH2	2:B:127:GLN:HB3	0.46	2.24	4	1
1:C:5:ALA:O	1:C:9:ASN:ND2	0.46	2.48	16	3
1:C:108:THR:O	1:C:110:ALA:N	0.46	2.48	5	4
1:A:83:LEU:C	1:A:83:LEU:CD1	0.46	2.79	7	1
1:C:122:HIS:CD2	1:C:122:HIS:H	0.46	2.28	8	1
2:B:57:ASN:C	2:B:57:ASN:HD22	0.46	2.14	9	1
2:D:15:TRP:HE1	2:D:72:SER:HG	0.46	1.51	9	1
1:C:39:THR:H	3:C:142:HEC:C3C	0.46	2.23	12	1
1:A:101:LEU:HD23	3:A:142:HEC:CBB	0.46	2.41	14	1
1:A:20:HIS:CB	1:A:24:TYR:CZ	0.46	2.98	16	1
1:A:100:LEU:O	1:A:104:CYS:N	0.46	2.46	19	1
2:B:107:GLY:C	2:B:109:VAL:N	0.46	2.68	19	1
1:A:3:SER:H	1:A:4:PRO:HD2	0.46	1.69	10	3
2:B:17:LYS:CD	2:B:17:LYS:N	0.46	2.78	15	4
1:C:3:SER:H	1:C:4:PRO:HD2	0.46	1.70	10	3
2:D:14:LEU:C	2:D:16:GLY:N	0.46	2.68	19	7
1:A:46:PHE:C	1:A:48:LEU:N	0.46	2.67	10	5
1:A:47:ASP:OD1	1:A:47:ASP:N	0.46	2.46	6	1
1:A:91:LEU:H	1:A:91:LEU:CD1	0.46	2.23	9	2
2:D:114:LEU:H	2:D:114:LEU:CD1	0.46	2.24	9	1
2:D:58:PRO:O	2:D:60:VAL:N	0.46	2.48	11	1
1:C:85:ASP:OD1	1:C:85:ASP:N	0.46	2.47	14	1
2:B:99:ASP:OD1	1:C:96:VAL:HG11	0.46	2.10	6	1
2:D:76:ALA:O	2:D:77:HIS:CD2	0.46	2.68	6	4
1:A:86:LEU:CG	3:A:142:HEC:CBD	0.46	2.93	7	1
2:B:20:VAL:C	2:B:22:GLU:N	0.46	2.68	15	2
1:C:101:LEU:HD23	3:C:142:HEC:CBB	0.46	2.41	14	1
1:C:101:LEU:HD21	3:C:142:HEC:CBB	0.46	2.30	15	2
1:A:24:TYR:CE2	1:A:112:HIS:CE1	0.46	3.03	16	1
1:A:40:LYS:O	1:A:41:THR:C	0.46	2.52	18	2
1:A:92:ARG:HH11	2:D:40:ARG:CD	0.46	2.18	18	1
1:A:84:SER:CB	1:A:136:LEU:O	0.46	2.64	20	1
2:D:112:CYS:SG	2:D:113:VAL:N	0.46	2.87	20	1
1:C:49:SER:O	1:C:50:HIS:O	0.46	2.32	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LYS:O	1:A:64:ASP:CB	0.46	2.63	11	9
2:B:32:LEU:CD2	2:B:38:THR:OG1	0.46	2.63	2	1
1:C:60:LYS:O	1:C:64:ASP:CB	0.46	2.63	11	9
1:A:46:PHE:O	1:A:46:PHE:CG	0.46	2.69	3	1
2:D:41:PHE:C	2:D:43:GLU:N	0.46	2.67	3	1
1:A:34:LEU:C	1:A:36:PHE:N	0.46	2.69	6	2
1:A:120:ALA:O	1:A:124:SER:OG	0.46	2.33	10	3
1:C:3:SER:N	1:C:4:PRO:HD2	0.46	2.26	10	6
2:B:93:CYS:SG	2:B:145:TYR:CE1	0.46	3.09	9	1
1:A:137:THR:O	1:A:137:THR:CG2	0.46	2.63	12	1
2:D:108:ASN:O	2:D:108:ASN:ND2	0.46	2.42	12	1
2:D:79:ASP:O	2:D:80:ASN:ND2	0.46	2.49	13	1
1:C:115:ALA:C	1:C:117:PHE:H	0.46	2.14	15	1
2:D:15:TRP:NE1	2:D:72:SER:OG	0.46	2.43	15	1
2:D:95:LYS:CA	2:D:97:HIS:HE2	0.46	2.24	15	1
3:B:147:HEC:HHC	3:B:147:HEC:HBB2	0.46	1.87	7	3
1:C:2:LEU:N	1:C:2:LEU:HD12	0.46	2.24	2	3
2:D:124:PRO:N	2:D:125:PRO:HD2	0.46	2.25	10	15
1:C:106:LEU:O	1:C:110:ALA:HB2	0.46	2.10	12	1
1:A:86:LEU:CD1	1:A:90:LYS:NZ	0.46	2.78	13	1
2:B:79:ASP:O	2:B:80:ASN:ND2	0.46	2.48	13	1
1:A:27:GLU:OE2	1:A:112:HIS:CE1	0.46	2.69	17	1
1:A:3:SER:H	1:A:6:ASP:CG	0.46	2.13	20	1
1:A:110:ALA:C	1:A:112:HIS:N	0.46	2.69	1	1
1:C:38:THR:O	1:C:40:LYS:N	0.46	2.49	16	3
1:C:45:HIS:O	1:C:45:HIS:ND1	0.46	2.48	5	2
2:D:77:HIS:O	2:D:78:LEU:C	0.46	2.54	6	1
1:C:89:HIS:O	1:C:90:LYS:O	0.46	2.33	15	3
1:A:92:ARG:O	1:A:93:VAL:CG1	0.46	2.64	13	1
1:C:92:ARG:O	1:C:93:VAL:CG1	0.46	2.64	13	1
2:D:20:VAL:C	2:D:22:GLU:N	0.46	2.68	15	2
2:B:40:ARG:HD2	1:C:92:ARG:HD2	0.46	1.70	18	1
1:C:101:LEU:CD1	3:C:142:HEC:C4B	0.46	2.91	19	1
1:C:84:SER:CB	1:C:136:LEU:O	0.46	2.64	20	1
1:A:76:MET:N	1:A:77:PRO:HD3	0.46	2.26	5	12
1:C:37:PRO:C	1:C:39:THR:N	0.46	2.68	10	11
2:D:119:GLY:O	2:D:122:PHE:N	0.46	2.47	19	2
2:B:139:ASN:OD1	2:D:146:HIS:C	0.46	2.53	6	1
1:A:118:THR:O	1:A:122:HIS:CD2	0.46	2.69	8	1
2:B:114:LEU:H	2:B:114:LEU:CD1	0.46	2.24	9	1
2:B:99:ASP:OD1	2:B:99:ASP:N	0.46	2.48	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:58:PRO:O	2:B:60:VAL:N	0.46	2.48	11	1
1:A:106:LEU:O	1:A:110:ALA:HB2	0.46	2.10	12	1
1:C:27:GLU:OE2	1:C:112:HIS:CE1	0.46	2.69	17	1
1:C:52:SER:O	1:C:53:ALA:C	0.46	2.54	18	1
1:C:7:LYS:O	1:C:11:LYS:HG2	0.46	2.11	1	2
1:A:5:ALA:O	1:A:9:ASN:ND2	0.46	2.49	14	3
2:B:97:HIS:HB3	1:C:38:THR:HG22	0.46	1.85	19	2
2:B:114:LEU:N	2:B:114:LEU:CD1	0.46	2.78	9	1
1:C:91:LEU:CD1	1:C:91:LEU:H	0.46	2.23	9	2
1:A:115:ALA:C	1:A:117:PHE:H	0.46	2.14	15	2
2:D:91:LEU:O	2:D:95:LYS:CB	0.46	2.63	9	7
2:D:40:ARG:C	2:D:42:PHE:N	0.46	2.69	15	2
2:D:96:LEU:O	2:D:96:LEU:HD13	0.46	2.11	4	1
1:A:46:PHE:O	1:A:48:LEU:CG	0.46	2.64	18	5
1:A:65:ALA:O	1:A:68:ASN:OD1	0.46	2.33	9	1
2:D:133:VAL:C	2:D:135:ALA:N	0.46	2.69	12	1
1:A:105:LEU:C	1:A:105:LEU:CD1	0.46	2.80	16	1
1:C:3:SER:H	1:C:6:ASP:CG	0.46	2.13	20	1
1:C:46:PHE:O	1:C:48:LEU:CG	0.46	2.64	18	5
1:A:5:ALA:C	1:A:7:LYS:N	0.46	2.67	12	3
2:B:15:TRP:HE1	2:B:72:SER:HG	0.46	1.46	15	2
2:B:142:ALA:O	2:B:145:TYR:N	0.46	2.48	12	1
1:C:137:THR:O	1:C:137:THR:CG2	0.46	2.63	12	1
3:B:147:HEC:CMC	2:D:31:LEU:HD21	0.46	2.41	15	1
1:A:94:ASP:CB	2:D:99:ASP:OD1	0.45	2.65	2	1
2:D:17:LYS:CD	2:D:17:LYS:N	0.45	2.79	13	7
2:B:110:LEU:HD23	2:B:110:LEU:C	0.45	2.32	12	3
2:D:57:ASN:C	2:D:57:ASN:HD22	0.45	2.14	9	1
1:C:84:SER:O	1:C:88:ALA:CB	0.45	2.64	13	4
1:C:86:LEU:CD1	1:C:90:LYS:NZ	0.45	2.78	13	1
3:B:147:HEC:HMC3	2:D:31:LEU:CD2	0.45	2.41	15	1
2:D:94:ASP:C	2:D:97:HIS:HE2	0.45	2.15	15	1
1:A:6:ASP:CG	1:A:127:LYS:HZ1	0.45	2.14	16	1
1:A:117:PHE:HA	2:B:30:ARG:HH22	0.45	1.71	17	1
1:A:7:LYS:O	1:A:11:LYS:HG2	0.45	2.11	8	2
2:D:106:LEU:HD11	3:D:147:HEC:CAB	0.45	2.29	2	1
1:C:58:HIS:C	1:C:58:HIS:CD2	0.45	2.88	3	1
2:B:96:LEU:O	2:B:96:LEU:HD13	0.45	2.11	4	1
1:C:65:ALA:O	1:C:68:ASN:OD1	0.45	2.33	9	1
2:D:6:GLU:CD	2:D:6:GLU:N	0.45	2.69	19	2
2:D:80:ASN:O	2:D:82:LYS:N	0.45	2.49	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:86:LEU:HD21	3:C:142:HEC:HBD2	0.45	1.88	13	1
2:D:111:VAL:HG12	2:D:130:TYR:CD1	0.45	2.47	14	1
1:C:108:THR:HG23	1:C:109:LEU:N	0.45	2.27	16	1
2:B:40:ARG:CZ	1:C:92:ARG:CD	0.45	2.94	18	1
1:A:38:THR:O	1:A:40:LYS:N	0.45	2.49	16	3
2:D:32:LEU:CD2	2:D:38:THR:OG1	0.45	2.64	2	1
2:B:135:ALA:HB3	2:D:146:HIS:HB3	0.45	1.88	3	1
1:A:88:ALA:O	1:A:89:HIS:CG	0.45	2.70	4	1
2:D:121:GLU:O	2:D:123:THR:N	0.45	2.48	9	1
2:B:146:HIS:N	2:B:146:HIS:HD1	0.45	2.09	11	1
2:D:20:VAL:HG12	2:D:20:VAL:O	0.45	2.10	11	2
2:D:42:PHE:CD1	3:D:147:HEC:C2B	0.45	2.98	12	1
1:A:92:ARG:HH21	2:D:40:ARG:CZ	0.45	2.12	15	1
2:B:40:ARG:C	2:B:42:PHE:N	0.45	2.69	15	1
1:C:78:ASN:ND2	1:C:79:ALA:N	0.45	2.64	17	1
2:B:6:GLU:CD	2:B:6:GLU:N	0.45	2.69	19	1
2:D:109:VAL:O	2:D:112:CYS:SG	0.45	2.71	20	1
1:A:91:LEU:O	1:A:92:ARG:C	0.45	2.53	12	2
2:B:124:PRO:N	2:B:125:PRO:HD2	0.45	2.27	16	15
1:C:1:VAL:O	1:C:2:LEU:O	0.45	2.35	2	4
1:C:2:LEU:CD2	1:C:128:PHE:CD2	0.45	3.00	9	1
1:C:18:GLY:O	1:C:19:ALA:CB	0.45	2.64	11	2
1:A:49:SER:CB	1:A:52:SER:OG	0.45	2.65	14	1
2:D:77:HIS:C	2:D:79:ASP:N	0.45	2.70	14	1
1:A:27:GLU:OE1	1:A:27:GLU:CA	0.45	2.63	15	1
2:B:40:ARG:C	1:C:92:ARG:NH1	0.45	2.69	17	1
1:C:86:LEU:C	1:C:86:LEU:CD1	0.45	2.82	19	1
1:C:122:HIS:CD2	2:D:34:VAL:HG13	0.45	2.47	19	1
2:D:96:LEU:C	2:D:97:HIS:CD2	0.45	2.90	19	1
1:A:1:VAL:O	1:A:2:LEU:O	0.45	2.35	1	3
1:C:34:LEU:CD1	1:C:35:SER:N	0.45	2.79	1	1
1:C:101:LEU:HD22	3:C:142:HEC:HAB	0.45	1.89	1	1
1:A:3:SER:N	1:A:4:PRO:HD2	0.45	2.26	9	6
2:D:144:LYS:C	2:D:146:HIS:H	0.45	2.15	19	5
2:B:143:HIS:CD2	2:B:143:HIS:O	0.45	2.70	16	2
1:C:48:LEU:HD22	1:C:49:SER:N	0.45	2.27	9	2
2:D:114:LEU:N	2:D:114:LEU:CD1	0.45	2.78	9	1
2:B:80:ASN:O	2:B:82:LYS:N	0.45	2.49	10	1
2:B:105:LEU:O	2:B:108:ASN:N	0.45	2.50	10	1
1:A:18:GLY:O	1:A:19:ALA:CB	0.45	2.64	11	1
1:A:84:SER:O	1:A:88:ALA:CB	0.45	2.65	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:117:PHE:CE2	2:D:116:HIS:NE2	0.45	2.58	13	1
1:A:93:VAL:O	2:D:40:ARG:NH1	0.45	2.49	14	1
3:B:147:HEC:C1C	2:D:106:LEU:CD1	0.45	2.77	15	1
1:A:127:LYS:CD	1:A:127:LYS:C	0.45	2.85	19	6
2:B:139:ASN:N	2:B:139:ASN:HD22	0.45	2.10	6	1
1:A:86:LEU:CD1	1:A:86:LEU:C	0.45	2.79	7	1
1:C:94:ASP:OD2	1:C:96:VAL:CG2	0.45	2.64	9	1
2:D:143:HIS:O	2:D:143:HIS:CD2	0.45	2.70	16	2
2:D:31:LEU:HD23	3:D:147:HEC:HBC2	0.45	1.89	10	1
2:D:47:ASP:OD1	2:D:47:ASP:N	0.45	2.49	10	1
2:B:13:ALA:C	2:B:15:TRP:N	0.45	2.67	15	3
2:B:111:VAL:HG12	2:B:130:TYR:CD1	0.45	2.47	14	1
2:D:90:GLU:O	2:D:94:ASP:CB	0.45	2.65	16	1
1:A:122:HIS:CD2	2:B:34:VAL:HG13	0.45	2.47	19	1
2:B:44:SER:C	2:B:46:GLY:N	0.45	2.69	3	6
1:A:58:HIS:C	1:A:58:HIS:CD2	0.45	2.88	3	1
2:B:8:LYS:O	2:B:10:ALA:N	0.45	2.50	19	6
2:B:36:PRO:C	2:B:38:THR:N	0.45	2.70	15	3
1:A:2:LEU:CD2	1:A:128:PHE:CD2	0.45	3.00	9	1
1:A:48:LEU:HD22	1:A:49:SER:N	0.45	2.27	9	2
1:C:50:HIS:ND1	1:C:50:HIS:C	0.45	2.70	9	1
2:D:93:CYS:SG	2:D:145:TYR:CE1	0.45	3.09	9	1
2:D:110:LEU:C	2:D:110:LEU:HD23	0.45	2.32	9	2
2:B:40:ARG:CZ	1:C:93:VAL:O	0.45	2.65	14	1
2:B:77:HIS:C	2:B:79:ASP:N	0.45	2.70	14	1
1:A:78:ASN:ND2	1:A:79:ALA:N	0.45	2.65	17	1
2:B:102:ASN:C	2:B:104:ARG:N	0.45	2.70	17	1
1:A:52:SER:O	1:A:53:ALA:C	0.45	2.54	18	1
2:B:8:LYS:CG	2:B:9:SER:N	0.45	2.80	19	1
1:C:61:LYS:HG3	3:C:142:HEC:CAA	0.45	2.42	19	1
1:A:34:LEU:CD1	1:A:35:SER:N	0.45	2.80	1	1
2:D:123:THR:O	2:D:127:GLN:OE1	0.45	2.35	1	1
2:D:97:HIS:O	2:D:97:HIS:CD2	0.45	2.70	2	2
2:B:111:VAL:CG1	2:B:130:TYR:CD1	0.45	3.00	5	1
1:A:94:ASP:OD2	1:A:96:VAL:CG2	0.45	2.64	9	1
2:B:47:ASP:N	2:B:47:ASP:OD1	0.45	2.49	10	1
1:C:33:PHE:CE1	3:C:142:HEC:C1D	0.45	3.00	12	1
2:D:42:PHE:CD1	3:D:147:HEC:C1B	0.45	3.00	12	1
1:C:49:SER:CB	1:C:52:SER:OG	0.45	2.65	14	1
1:A:92:ARG:HH21	2:D:40:ARG:HE	0.45	0.56	15	1
1:A:109:LEU:C	1:A:109:LEU:CD1	0.45	2.81	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:127:GLN:O	2:D:131:GLN:OE1	0.45	2.35	16	1
2:B:146:HIS:HD2	2:D:139:ASN:OD1	0.45	1.94	17	1
2:B:101:GLU:O	2:B:102:ASN:OD1	0.45	2.35	18	1
2:B:96:LEU:C	2:B:97:HIS:CD2	0.45	2.90	19	1
1:A:100:LEU:O	1:A:102:SER:N	0.45	2.50	20	1
2:B:83:GLY:O	2:B:86:ALA:N	0.45	2.43	4	1
2:B:96:LEU:HD12	2:B:98:VAL:CG2	0.45	2.42	6	1
1:C:118:THR:O	1:C:122:HIS:CD2	0.45	2.69	8	1
2:B:133:VAL:C	2:B:135:ALA:N	0.45	2.68	12	1
1:C:46:PHE:CD1	3:C:142:HEC:CMA	0.45	2.88	12	1
1:A:33:PHE:O	1:A:36:PHE:O	0.45	2.35	14	1
3:B:147:HEC:C2C	2:D:106:LEU:HD12	0.45	2.41	15	1
2:B:127:GLN:O	2:B:131:GLN:OE1	0.45	2.35	16	1
1:C:117:PHE:HA	2:D:30:ARG:HH22	0.45	1.71	17	1
2:D:101:GLU:O	2:D:102:ASN:OD1	0.45	2.35	18	1
1:A:115:ALA:O	1:A:121:VAL:CG2	0.45	2.60	1	1
2:B:123:THR:O	2:B:127:GLN:OE1	0.45	2.35	1	1
1:A:137:THR:O	1:A:138:SER:O	0.45	2.36	3	3
1:A:68:ASN:HD21	1:A:79:ALA:CB	0.45	2.25	5	1
2:B:111:VAL:CG1	2:B:130:TYR:CE1	0.45	3.00	5	1
2:D:67:VAL:CG2	3:D:147:HEC:NA	0.45	2.80	9	1
2:B:37:TRP:CD1	2:B:38:THR:HG23	0.45	2.47	10	2
1:C:27:GLU:OE1	1:C:27:GLU:CA	0.45	2.62	15	1
1:A:101:LEU:CD1	3:A:142:HEC:C4B	0.45	2.91	19	1
2:B:56:GLY:O	2:B:57:ASN:HB2	0.45	2.12	19	1
1:C:100:LEU:O	1:C:102:SER:N	0.45	2.50	20	1
2:D:127:GLN:O	2:D:130:TYR:N	0.44	2.51	1	2
2:D:96:LEU:HD12	2:D:98:VAL:HG23	0.44	1.87	6	2
2:B:102:ASN:ND2	3:B:147:HEC:HMC2	0.44	2.27	7	1
2:B:114:LEU:HD12	2:B:114:LEU:H	0.44	1.71	9	1
2:D:21:ASP:N	2:D:21:ASP:OD1	0.44	2.50	9	1
1:A:17:VAL:O	1:A:18:GLY:O	0.44	2.35	11	3
2:B:97:HIS:CE1	1:C:41:THR:HG22	0.44	2.48	11	1
1:C:48:LEU:CD1	3:C:142:HEC:HAA1	0.44	2.42	12	1
2:D:36:PRO:C	3:D:147:HEC:C2C	0.44	2.82	12	1
1:A:137:THR:O	1:A:138:SER:CB	0.44	2.63	15	1
2:B:114:LEU:O	2:B:116:HIS:N	0.44	2.50	20	2
2:B:39:GLN:OE1	2:B:39:GLN:O	0.44	2.36	16	1
1:A:92:ARG:O	1:A:93:VAL:C	0.44	2.55	17	2
2:B:102:ASN:O	2:B:104:ARG:N	0.44	2.50	17	1
2:B:67:VAL:HG13	3:B:147:HEC:C3B	0.44	2.34	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:8:LYS:CG	2:D:9:SER:N	0.44	2.79	19	1
2:D:142:ALA:C	2:D:144:LYS:N	0.44	2.69	20	1
1:A:62:VAL:HG12	1:A:63:ALA:N	0.44	2.28	1	3
1:A:127:LYS:C	1:A:129:LEU:N	0.44	2.70	2	7
3:A:142:HEC:HMB1	3:A:142:HEC:CBB	0.44	2.31	11	6
1:C:60:LYS:O	1:C:64:ASP:CG	0.44	2.56	6	2
1:C:34:LEU:C	1:C:36:PHE:N	0.44	2.69	6	3
2:D:96:LEU:HD12	2:D:98:VAL:CG2	0.44	2.42	6	1
2:B:21:ASP:C	2:B:65:LYS:HZ3	0.44	2.15	10	1
1:C:32:MET:CE	3:C:142:HEC:C3B	0.44	2.95	12	1
1:A:94:ASP:O	1:A:97:ASN:OD1	0.44	2.35	16	1
2:B:97:HIS:O	2:B:97:HIS:CD2	0.44	2.70	2	2
1:C:94:ASP:C	1:C:96:VAL:N	0.44	2.71	4	6
2:D:40:ARG:O	2:D:42:PHE:N	0.44	2.50	15	2
1:C:88:ALA:O	1:C:89:HIS:CG	0.44	2.70	4	1
1:A:60:LYS:O	1:A:64:ASP:CG	0.44	2.56	6	3
2:B:97:HIS:CG	1:C:38:THR:HG22	0.44	2.38	7	1
1:C:120:ALA:O	1:C:124:SER:OG	0.44	2.33	10	5
2:B:21:ASP:N	2:B:21:ASP:OD1	0.44	2.50	9	2
2:B:42:PHE:CE1	2:B:45:PHE:CZ	0.44	3.06	16	1
2:B:146:HIS:CE1	2:D:135:ALA:HB3	0.44	2.47	17	1
2:D:102:ASN:O	2:D:104:ARG:N	0.44	2.50	17	1
2:B:132:LYS:NZ	2:B:132:LYS:CB	0.44	2.80	18	1
2:B:95:LYS:O	2:B:97:HIS:CD2	0.44	2.70	19	1
1:C:110:ALA:C	1:C:112:HIS:N	0.44	2.69	1	1
2:B:119:GLY:C	2:B:121:GLU:H	0.44	2.16	16	2
2:B:106:LEU:HD13	3:B:147:HEC:HAB	0.44	1.85	3	2
2:D:8:LYS:O	2:D:10:ALA:N	0.44	2.50	19	7
2:B:146:HIS:ND1	2:B:146:HIS:C	0.44	2.71	7	1
1:A:94:ASP:O	1:A:97:ASN:ND2	0.44	2.50	8	1
2:B:101:GLU:C	2:B:102:ASN:ND2	0.44	2.71	8	1
1:C:48:LEU:CD1	1:C:48:LEU:N	0.44	2.80	8	1
2:B:82:LYS:HZ2	2:B:143:HIS:CD2	0.44	2.31	11	2
1:C:33:PHE:O	1:C:36:PHE:O	0.44	2.35	14	1
1:C:32:MET:C	1:C:34:LEU:N	0.44	2.69	16	1
2:D:68:LEU:C	2:D:68:LEU:HD23	0.44	2.33	17	1
2:D:132:LYS:NZ	2:D:132:LYS:CB	0.44	2.80	18	1
2:B:67:VAL:CG1	3:B:147:HEC:C3B	0.44	2.96	19	1
1:C:2:LEU:HD12	1:C:6:ASP:OD2	0.44	2.12	19	1
1:C:132:VAL:O	1:C:136:LEU:HD13	0.44	2.13	20	1
1:C:137:THR:O	1:C:138:SER:O	0.44	2.36	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:THR:OG1	1:A:121:VAL:CB	0.44	2.66	20	2
1:A:68:ASN:HD21	1:A:80:LEU:HD21	0.44	1.73	9	1
2:B:67:VAL:CG2	3:B:147:HEC:NA	0.44	2.80	9	1
2:B:121:GLU:O	2:B:123:THR:N	0.44	2.48	9	1
1:C:34:LEU:C	1:C:34:LEU:CD1	0.44	2.82	9	1
2:B:31:LEU:HD23	3:B:147:HEC:HBC2	0.44	1.89	10	1
2:B:58:PRO:C	2:B:60:VAL:N	0.44	2.71	11	1
2:D:2:HIS:CD2	2:D:2:HIS:C	0.44	2.90	14	1
2:D:56:GLY:O	2:D:57:ASN:ND2	0.44	2.51	19	1
1:A:74:ASP:O	1:A:75:ASP:CG	0.44	2.56	18	5
2:B:127:GLN:OE1	2:B:127:GLN:N	0.44	2.51	1	1
1:C:74:ASP:O	1:C:75:ASP:CG	0.44	2.56	18	5
1:C:127:LYS:C	1:C:129:LEU:N	0.44	2.70	2	7
2:D:44:SER:C	2:D:46:GLY:N	0.44	2.69	3	6
1:C:87:HIS:O	1:C:90:LYS:O	0.44	2.36	5	1
2:B:144:LYS:C	2:B:146:HIS:H	0.44	2.15	19	6
1:C:94:ASP:O	1:C:97:ASN:ND2	0.44	2.50	8	1
2:B:67:VAL:HA	3:B:147:HEC:HBB	0.44	1.89	9	1
1:C:29:LEU:HD13	1:C:58:HIS:CD2	0.44	2.48	14	1
2:B:90:GLU:O	2:B:94:ASP:CB	0.44	2.65	16	1
2:D:95:LYS:O	2:D:97:HIS:CD2	0.44	2.70	19	1
1:A:110:ALA:C	1:A:112:HIS:H	0.44	2.15	1	1
1:C:62:VAL:HG12	1:C:63:ALA:N	0.44	2.28	1	2
1:C:115:ALA:HB1	1:C:121:VAL:HG13	0.44	1.89	1	3
2:B:40:ARG:O	2:B:42:PHE:N	0.44	2.50	15	2
1:A:94:ASP:OD1	1:A:94:ASP:N	0.44	2.51	3	1
1:A:106:LEU:CD1	1:A:122:HIS:CE1	0.44	2.99	4	1
1:C:68:ASN:HD21	1:C:79:ALA:CB	0.44	2.25	5	1
2:D:111:VAL:CG1	2:D:130:TYR:CD1	0.44	3.00	5	1
2:B:99:ASP:O	2:B:102:ASN:OD1	0.44	2.36	6	2
1:C:113:LEU:C	1:C:113:LEU:CD1	0.44	2.86	12	2
1:A:33:PHE:CZ	1:A:46:PHE:CZ	0.44	3.06	9	1
1:A:50:HIS:ND1	1:A:50:HIS:C	0.44	2.70	9	1
2:B:130:TYR:O	2:B:133:VAL:HG12	0.44	2.13	9	1
1:C:68:ASN:HD21	1:C:80:LEU:HD21	0.44	1.73	9	1
1:C:78:ASN:O	1:C:81:SER:OG	0.44	2.36	9	1
1:A:84:SER:O	1:A:88:ALA:HB2	0.44	2.12	10	3
2:D:37:TRP:CD1	2:D:38:THR:HG23	0.44	2.47	10	2
1:C:89:HIS:O	1:C:90:LYS:C	0.44	2.56	15	2
1:A:98:PHE:CZ	1:A:136:LEU:HD23	0.44	2.48	15	1
2:B:2:HIS:CE1	2:D:146:HIS:CD2	0.44	2.83	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ALA:HB3	3:A:142:HEC:HMB3	0.44	1.90	20	1
1:A:52:SER:C	1:A:54:GLN:H	0.44	2.16	1	4
1:A:101:LEU:HD22	3:A:142:HEC:HAB	0.44	1.89	1	1
1:C:52:SER:C	1:C:54:GLN:H	0.44	2.15	1	5
1:A:94:ASP:C	1:A:96:VAL:N	0.44	2.71	4	5
1:C:127:LYS:CG	1:C:128:PHE:N	0.44	2.81	4	11
2:D:102:ASN:ND2	3:D:147:HEC:HMC2	0.44	2.27	7	1
2:D:101:GLU:C	2:D:102:ASN:ND2	0.44	2.71	8	1
2:B:57:ASN:ND2	2:B:57:ASN:C	0.44	2.71	9	1
2:D:57:ASN:ND2	2:D:57:ASN:C	0.44	2.71	9	1
2:D:130:TYR:O	2:D:133:VAL:HG12	0.44	2.13	9	1
2:B:145:TYR:O	2:B:146:HIS:O	0.44	2.36	10	2
1:C:103:HIS:CB	2:D:108:ASN:ND2	0.44	2.80	10	1
2:D:145:TYR:O	2:D:146:HIS:O	0.44	2.36	10	2
1:A:121:VAL:CG1	1:A:122:HIS:CE1	0.44	3.01	12	1
2:B:108:ASN:O	2:B:112:CYS:SG	0.44	2.71	12	1
2:D:110:LEU:O	2:D:113:VAL:N	0.44	2.51	12	1
2:D:114:LEU:O	2:D:116:HIS:N	0.44	2.50	20	2
1:A:132:VAL:O	1:A:136:LEU:HD13	0.44	2.13	20	1
1:A:27:GLU:CG	1:A:108:THR:OG1	0.44	2.66	1	1
2:B:33:VAL:CG1	2:B:34:VAL:H	0.44	2.23	3	1
2:B:97:HIS:ND1	1:C:37:PRO:O	0.44	2.51	3	1
2:D:33:VAL:CG1	2:D:34:VAL:H	0.44	2.23	3	1
2:B:4:THR:O	2:B:7:GLU:N	0.44	2.46	16	3
2:D:139:ASN:N	2:D:139:ASN:HD22	0.44	2.10	6	1
1:A:57:GLY:O	1:A:61:LYS:CE	0.44	2.66	9	1
1:C:68:ASN:ND2	1:C:80:LEU:HD21	0.44	2.28	9	1
2:D:42:PHE:CE2	3:D:147:HEC:CMB	0.44	2.91	12	1
2:B:2:HIS:CD2	2:B:2:HIS:C	0.44	2.90	14	1
2:B:82:LYS:NZ	2:B:143:HIS:ND1	0.44	2.66	16	1
2:D:102:ASN:C	2:D:104:ARG:N	0.44	2.70	17	1
2:B:67:VAL:HA	3:B:147:HEC:C4A	0.44	2.43	19	1
1:A:115:ALA:HB1	1:A:121:VAL:HG13	0.43	1.90	19	3
1:A:127:LYS:HG3	1:A:128:PHE:N	0.43	2.28	3	3
1:C:127:LYS:HG3	1:C:128:PHE:N	0.43	2.28	19	3
2:D:19:ASN:C	2:D:21:ASP:H	0.43	2.16	11	4
1:A:127:LYS:O	1:A:129:LEU:N	0.43	2.51	2	4
1:C:108:THR:C	1:C:110:ALA:N	0.43	2.70	5	3
2:D:99:ASP:O	2:D:102:ASN:OD1	0.43	2.36	13	2
1:A:69:ALA:CB	1:A:76:MET:SD	0.43	3.06	10	2
2:B:19:ASN:C	2:B:21:ASP:H	0.43	2.16	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:73:ASP:OD2	2:B:84:THR:OG1	0.43	2.37	15	1
2:D:32:LEU:HB3	3:D:147:HEC:CMB	0.43	2.39	15	1
1:A:32:MET:C	1:A:34:LEU:N	0.43	2.69	16	1
2:B:90:GLU:O	2:B:94:ASP:N	0.43	2.45	16	1
2:D:42:PHE:CE1	2:D:45:PHE:CZ	0.43	3.06	16	1
2:D:67:VAL:CG1	3:D:147:HEC:C3B	0.43	2.96	19	1
1:C:76:MET:N	1:C:77:PRO:HD3	0.43	2.27	10	13
1:A:127:LYS:CG	1:A:128:PHE:N	0.43	2.81	4	9
2:D:82:LYS:N	2:D:82:LYS:CD	0.43	2.81	18	2
1:C:82:ALA:O	1:C:83:LEU:C	0.43	2.57	13	11
1:A:108:THR:C	1:A:110:ALA:N	0.43	2.70	5	2
2:D:111:VAL:CG1	2:D:130:TYR:CE1	0.43	3.00	5	1
2:D:41:PHE:C	2:D:42:PHE:CD1	0.43	2.91	6	2
2:D:102:ASN:C	2:D:102:ASN:HD22	0.43	2.16	7	1
1:A:73:VAL:O	1:A:74:ASP:OD1	0.43	2.37	16	4
1:A:23:GLU:O	1:A:27:GLU:OE1	0.43	2.36	9	1
2:B:67:VAL:HG13	3:B:147:HEC:HMB3	0.43	1.90	9	1
2:B:75:LEU:HD12	2:B:75:LEU:H	0.43	1.73	16	2
1:C:2:LEU:CD2	1:C:6:ASP:OD1	0.43	2.67	9	1
1:C:33:PHE:CZ	1:C:46:PHE:CZ	0.43	3.06	9	1
1:C:17:VAL:O	1:C:18:GLY:O	0.43	2.36	16	3
1:A:115:ALA:CB	1:A:122:HIS:NE2	0.43	2.81	12	1
1:A:92:ARG:NH2	2:D:40:ARG:CG	0.43	2.81	15	1
2:D:73:ASP:OD2	2:D:84:THR:OG1	0.43	2.36	15	1
1:A:88:ALA:C	1:A:90:LYS:H	0.43	2.16	17	1
1:C:56:LYS:CG	1:C:57:GLY:N	0.43	2.81	19	1
2:D:56:GLY:O	2:D:57:ASN:HB2	0.43	2.12	19	1
1:C:110:ALA:C	1:C:112:HIS:H	0.43	2.15	1	1
1:C:127:LYS:O	1:C:129:LEU:N	0.43	2.51	2	3
2:B:77:HIS:O	2:B:78:LEU:C	0.43	2.54	6	1
1:A:68:ASN:ND2	1:A:80:LEU:HD21	0.43	2.28	9	1
2:B:43:GLU:CD	2:B:44:SER:H	0.43	2.17	9	1
1:A:38:THR:O	1:A:41:THR:CG2	0.43	2.67	15	2
2:B:41:PHE:O	2:B:42:PHE:CG	0.43	2.72	11	1
2:B:123:THR:C	2:B:127:GLN:HE22	0.43	2.17	11	1
1:A:118:THR:O	1:A:121:VAL:HG12	0.43	2.13	12	2
1:C:121:VAL:CG1	1:C:122:HIS:CE1	0.43	3.01	12	1
1:A:108:THR:HG23	1:A:109:LEU:N	0.43	2.27	16	1
1:C:94:ASP:O	1:C:97:ASN:OD1	0.43	2.36	16	1
2:D:79:ASP:OD1	2:D:80:ASN:N	0.43	2.51	17	1
2:B:56:GLY:O	2:B:57:ASN:ND2	0.43	2.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:ALA:O	1:A:121:VAL:HG11	0.43	2.13	20	1
1:C:115:ALA:O	1:C:121:VAL:HG11	0.43	2.13	20	1
2:B:131:GLN:H	2:B:131:GLN:CD	0.43	2.16	5	1
1:C:118:THR:OG1	1:C:121:VAL:CB	0.43	2.66	20	2
1:A:113:LEU:C	1:A:113:LEU:CD1	0.43	2.86	12	2
1:C:134:THR:O	1:C:137:THR:OG1	0.43	2.36	7	1
2:D:36:PRO:C	2:D:38:THR:N	0.43	2.70	15	2
1:C:38:THR:O	1:C:41:THR:CG2	0.43	2.67	15	2
1:C:84:SER:O	1:C:88:ALA:HB2	0.43	2.12	10	3
1:C:52:SER:OG	1:C:55:VAL:HG23	0.43	2.14	11	1
1:C:31:ARG:CG	1:C:31:ARG:HH11	0.43	2.26	12	1
1:C:32:MET:SD	3:C:142:HEC:CHC	0.43	3.06	12	1
2:D:31:LEU:O	2:D:35:TYR:O	0.43	2.37	12	1
2:D:42:PHE:HB3	3:D:147:HEC:HMA2	0.43	1.66	12	1
1:A:29:LEU:HD13	1:A:58:HIS:CD2	0.43	2.48	14	1
2:D:26:GLU:O	2:D:28:LEU:N	0.43	2.52	14	1
1:A:85:ASP:O	1:A:89:HIS:CB	0.43	2.67	16	1
1:C:92:ARG:O	1:C:93:VAL:C	0.43	2.55	17	2
1:A:84:SER:OG	1:A:135:VAL:O	0.43	2.37	18	1
2:D:90:GLU:O	2:D:94:ASP:OD2	0.43	2.36	18	1
1:A:2:LEU:HD12	1:A:6:ASP:OD2	0.43	2.12	19	1
2:B:110:LEU:HD23	2:B:110:LEU:O	0.43	2.13	3	3
1:C:27:GLU:CG	1:C:108:THR:OG1	0.43	2.66	1	1
1:A:82:ALA:O	1:A:83:LEU:C	0.43	2.57	13	13
1:A:130:ALA:O	1:A:134:THR:OG1	0.43	2.34	8	1
1:C:23:GLU:O	1:C:27:GLU:OE1	0.43	2.36	9	1
2:D:75:LEU:HD12	2:D:75:LEU:H	0.43	1.73	16	2
2:D:134:VAL:O	2:D:136:GLY:N	0.43	2.51	19	3
1:A:31:ARG:NH1	1:A:31:ARG:CG	0.43	2.80	12	1
2:B:14:LEU:O	2:B:17:LYS:N	0.43	2.52	12	1
2:B:110:LEU:O	2:B:113:VAL:N	0.43	2.49	13	2
1:C:115:ALA:CB	1:C:122:HIS:NE2	0.43	2.81	12	1
2:D:82:LYS:NZ	2:D:143:HIS:ND1	0.43	2.66	16	1
1:A:98:PHE:N	1:A:98:PHE:CD1	0.43	2.85	17	1
2:B:79:ASP:OD1	2:B:80:ASN:N	0.43	2.51	17	1
2:B:40:ARG:HD2	1:C:92:ARG:NE	0.43	2.22	18	1
2:D:4:THR:OG1	2:D:7:GLU:OE2	0.43	2.35	19	1
2:B:127:GLN:O	2:B:130:TYR:N	0.43	2.51	1	1
1:C:11:LYS:CD	1:C:11:LYS:H	0.43	2.27	15	2
2:D:23:VAL:O	2:D:27:ALA:CB	0.43	2.67	5	1
2:D:102:ASN:O	2:D:105:LEU:N	0.43	2.51	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:57:ASN:ND2	2:B:60:VAL:H	0.43	2.12	9	1
2:D:57:ASN:ND2	2:D:60:VAL:H	0.43	2.12	9	1
1:A:6:ASP:OD2	1:A:127:LYS:CE	0.43	2.67	10	1
1:C:6:ASP:OD2	1:C:127:LYS:CE	0.43	2.67	10	1
2:D:19:ASN:HD22	2:D:19:ASN:N	0.43	2.12	11	1
2:B:145:TYR:O	2:B:145:TYR:CD2	0.43	2.71	12	1
2:D:36:PRO:O	3:D:147:HEC:C1C	0.43	2.67	12	1
2:D:142:ALA:O	2:D:145:TYR:N	0.43	2.48	12	1
1:A:49:SER:O	1:A:52:SER:OG	0.43	2.36	14	1
3:B:147:HEC:HBC2	2:D:31:LEU:HD23	0.43	1.91	15	1
1:A:14:TRP:NE1	1:A:67:THR:OG1	0.43	2.49	17	1
2:B:134:VAL:O	2:B:136:GLY:N	0.43	2.51	19	2
1:C:71:ALA:C	1:C:72:HIS:CG	0.43	2.92	17	1
1:A:58:HIS:C	1:A:58:HIS:HD1	0.43	2.17	18	1
1:A:80:LEU:N	1:A:80:LEU:CD1	0.43	2.81	18	1
2:B:56:GLY:O	2:B:57:ASN:CG	0.43	2.57	19	1
2:B:76:ALA:O	2:B:77:HIS:ND1	0.43	2.51	19	2
2:D:36:PRO:O	2:D:39:GLN:N	0.43	2.44	19	1
2:D:110:LEU:HD23	2:D:110:LEU:O	0.43	2.13	3	3
2:B:82:LYS:N	2:B:82:LYS:CD	0.43	2.81	18	2
2:B:104:ARG:O	2:B:108:ASN:OD1	0.43	2.37	3	3
1:C:94:ASP:OD1	1:C:94:ASP:N	0.43	2.51	3	1
2:B:127:GLN:HE22	2:B:131:GLN:CG	0.43	2.27	4	1
2:B:119:GLY:O	2:B:121:GLU:N	0.43	2.52	5	1
1:A:96:VAL:CG1	2:D:99:ASP:OD1	0.43	2.66	6	1
1:C:1:VAL:HG12	1:C:1:VAL:O	0.43	2.13	6	1
2:B:102:ASN:O	2:B:105:LEU:N	0.43	2.51	7	1
2:B:131:GLN:O	2:B:135:ALA:N	0.43	2.49	9	1
2:D:67:VAL:HA	3:D:147:HEC:HHB	0.43	1.89	9	1
1:A:52:SER:OG	1:A:55:VAL:HG23	0.43	2.14	11	1
2:D:41:PHE:O	2:D:42:PHE:CG	0.43	2.72	11	1
2:B:17:LYS:N	2:B:17:LYS:HD2	0.43	2.29	15	1
2:B:85:PHE:CZ	2:B:137:VAL:HG13	0.43	2.49	16	1
2:B:104:ARG:NH2	2:D:146:HIS:C	0.43	2.72	17	1
1:C:75:ASP:O	1:C:78:ASN:OD1	0.43	2.37	17	1
1:C:2:LEU:C	1:C:3:SER:OG	0.43	2.57	18	1
1:C:84:SER:OG	1:C:135:VAL:O	0.43	2.37	18	1
1:A:100:LEU:C	1:A:102:SER:N	0.43	2.72	20	1
1:C:11:LYS:NZ	1:C:70:VAL:HG13	0.43	2.29	1	1
1:A:1:VAL:CG2	1:A:131:SER:OG	0.43	2.67	4	1
2:B:45:PHE:O	2:B:46:GLY:O	0.43	2.37	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:119:GLY:C	2:B:121:GLU:N	0.43	2.72	5	1
2:D:119:GLY:O	2:D:121:GLU:N	0.43	2.52	5	1
2:B:41:PHE:C	2:B:42:PHE:CD1	0.43	2.91	6	2
2:B:102:ASN:HD22	2:B:102:ASN:C	0.43	2.16	7	1
1:A:78:ASN:O	1:A:81:SER:OG	0.43	2.36	9	1
1:C:14:TRP:NE1	1:C:67:THR:OG1	0.43	2.49	17	2
2:D:50:THR:O	2:D:52:ASP:N	0.43	2.52	9	1
1:C:6:ASP:OD1	1:C:6:ASP:N	0.43	2.50	10	1
2:D:26:GLU:O	2:D:30:ARG:NH1	0.43	2.52	11	1
2:D:14:LEU:O	2:D:17:LYS:N	0.43	2.52	12	1
1:A:89:HIS:O	1:A:90:LYS:C	0.43	2.56	15	2
1:A:118:THR:OG1	1:A:121:VAL:HG23	0.43	2.14	15	1
1:C:98:PHE:CZ	1:C:136:LEU:HD23	0.43	2.48	15	1
2:B:90:GLU:O	2:B:94:ASP:OD2	0.43	2.36	18	1
2:D:67:VAL:HA	3:D:147:HEC:C4A	0.43	2.43	19	1
2:D:106:LEU:HD23	2:D:106:LEU:O	0.43	2.13	3	1
1:C:1:VAL:CG2	1:C:131:SER:OG	0.43	2.67	4	1
1:C:64:ASP:O	1:C:68:ASN:N	0.43	2.41	4	1
1:A:96:VAL:HG21	2:D:99:ASP:CG	0.43	2.34	5	1
1:A:103:HIS:CD2	2:B:108:ASN:ND2	0.43	2.86	5	1
2:B:23:VAL:O	2:B:27:ALA:CB	0.43	2.67	5	1
1:C:103:HIS:CD2	2:D:108:ASN:ND2	0.43	2.86	5	1
1:C:127:LYS:HD2	1:C:128:PHE:N	0.43	2.29	7	2
1:C:73:VAL:O	1:C:74:ASP:OD1	0.43	2.37	16	3
1:C:57:GLY:O	1:C:61:LYS:CE	0.43	2.66	9	1
1:A:48:LEU:N	1:A:48:LEU:CD1	0.43	2.69	11	1
1:A:118:THR:O	1:A:118:THR:OG1	0.43	2.36	18	4
2:B:37:TRP:O	2:B:39:GLN:N	0.43	2.51	14	1
1:C:85:ASP:O	1:C:89:HIS:CB	0.43	2.67	16	1
2:D:82:LYS:NZ	2:D:143:HIS:CG	0.43	2.87	16	1
2:D:85:PHE:CZ	2:D:137:VAL:HG13	0.43	2.49	16	1
1:C:130:ALA:O	1:C:134:THR:CB	0.43	2.67	20	1
1:A:17:VAL:HG11	1:A:21:ALA:HB2	0.43	1.91	1	1
2:D:5:PRO:O	2:D:9:SER:OG	0.43	2.34	6	2
1:A:46:PHE:O	1:A:47:ASP:OD1	0.43	2.37	2	1
1:A:47:ASP:OD1	1:A:47:ASP:O	0.43	2.37	2	1
2:D:104:ARG:O	2:D:108:ASN:ND2	0.43	2.52	2	1
2:D:119:GLY:C	2:D:121:GLU:H	0.43	2.16	16	2
2:B:106:LEU:CD2	2:B:106:LEU:C	0.43	2.86	3	1
2:D:127:GLN:HE22	2:D:131:GLN:CG	0.43	2.27	4	1
2:D:42:PHE:CG	2:D:43:GLU:N	0.43	2.87	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:17:LYS:H	2:D:17:LYS:HD2	0.43	1.74	8	1
2:D:21:ASP:OD1	2:D:21:ASP:N	0.43	2.51	8	1
1:A:2:LEU:CD2	1:A:6:ASP:OD1	0.43	2.67	9	1
1:A:27:GLU:CD	1:A:27:GLU:N	0.43	2.72	9	1
1:A:91:LEU:HD12	1:A:91:LEU:H	0.43	1.71	9	2
2:D:105:LEU:O	2:D:108:ASN:N	0.43	2.50	10	1
2:B:3:LEU:CD1	2:B:3:LEU:N	0.43	2.78	12	1
1:C:118:THR:O	1:C:121:VAL:HG12	0.43	2.13	12	2
1:C:118:THR:OG1	1:C:121:VAL:HG23	0.43	2.14	15	1
2:D:100:PRO:C	2:D:102:ASN:HD22	0.43	2.17	15	1
2:D:114:LEU:C	2:D:116:HIS:N	0.43	2.71	20	2
1:A:71:ALA:C	1:A:72:HIS:CG	0.43	2.92	17	1
1:A:75:ASP:O	1:A:78:ASN:OD1	0.43	2.37	17	1
2:B:68:LEU:C	2:B:68:LEU:HD23	0.43	2.33	17	1
2:B:6:GLU:N	2:B:6:GLU:OE1	0.43	2.52	19	1
1:A:130:ALA:O	1:A:134:THR:CB	0.43	2.67	20	1
1:C:32:MET:HE3	3:C:142:HEC:CBC	0.42	2.44	5	2
2:D:96:LEU:O	2:D:97:HIS:C	0.42	2.57	20	6
1:A:98:PHE:CD1	1:A:99:LYS:N	0.42	2.87	3	1
2:B:48:LEU:O	2:B:49:SER:C	0.42	2.58	10	2
2:B:146:HIS:ND1	2:D:135:ALA:HB1	0.42	2.28	3	1
1:A:117:PHE:CE1	2:B:116:HIS:CE1	0.42	3.07	4	1
2:B:42:PHE:CG	2:B:43:GLU:N	0.42	2.87	5	2
3:C:142:HEC:HBB3	3:C:142:HEC:CMB	0.42	2.39	6	2
2:B:96:LEU:O	2:B:97:HIS:C	0.42	2.57	20	5
1:C:63:ALA:O	1:C:67:THR:OG1	0.42	2.30	9	2
2:D:117:HIS:ND1	2:D:117:HIS:O	0.42	2.49	10	1
1:C:31:ARG:CG	1:C:31:ARG:NH1	0.42	2.80	12	1
2:B:80:ASN:ND2	2:B:80:ASN:O	0.42	2.52	14	1
2:D:80:ASN:ND2	2:D:80:ASN:O	0.42	2.52	14	1
2:B:82:LYS:HZ1	2:D:82:LYS:HZ1	0.42	0.50	15	1
2:B:82:LYS:NZ	2:B:143:HIS:CG	0.42	2.87	16	1
1:A:61:LYS:HB3	3:A:142:HEC:CMA	0.42	2.44	17	2
1:A:56:LYS:CG	1:A:57:GLY:N	0.42	2.81	19	1
2:B:104:ARG:O	2:B:108:ASN:ND2	0.42	2.52	2	1
1:A:31:ARG:O	1:A:35:SER:OG	0.42	2.37	4	1
1:A:87:HIS:O	1:A:90:LYS:O	0.42	2.36	5	1
2:B:80:ASN:OD1	2:B:80:ASN:O	0.42	2.38	8	1
1:C:9:ASN:C	1:C:124:SER:OG	0.42	2.57	8	1
2:D:42:PHE:CZ	2:D:45:PHE:CD2	0.42	3.07	8	1
1:C:69:ALA:CB	1:C:76:MET:SD	0.42	3.07	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:53:ALA:O	1:C:54:GLN:C	0.42	2.58	19	2
2:B:26:GLU:O	2:B:28:LEU:N	0.42	2.52	14	1
2:B:77:HIS:C	2:B:79:ASP:H	0.42	2.17	14	2
2:D:37:TRP:C	2:D:39:GLN:H	0.42	2.17	14	1
2:B:20:VAL:C	2:B:22:GLU:H	0.42	2.18	15	1
2:B:40:ARG:C	2:B:42:PHE:H	0.42	2.17	15	1
1:C:98:PHE:CD1	1:C:98:PHE:N	0.42	2.85	17	1
1:C:107:VAL:HG11	2:D:127:GLN:NE2	0.42	2.29	17	1
2:B:67:VAL:CG1	3:B:147:HEC:NB	0.42	2.76	19	1
2:D:76:ALA:O	2:D:77:HIS:ND1	0.42	2.51	19	2
1:A:7:LYS:O	1:A:8:THR:C	0.42	2.58	1	3
1:A:41:THR:CB	2:D:94:ASP:O	0.42	2.67	1	1
1:C:46:PHE:O	1:C:47:ASP:OD1	0.42	2.37	2	1
2:D:131:GLN:H	2:D:131:GLN:CD	0.42	2.16	5	1
2:B:112:CYS:O	2:B:116:HIS:CE1	0.42	2.72	9	1
2:B:19:ASN:N	2:B:19:ASN:HD22	0.42	2.12	11	1
2:D:58:PRO:C	2:D:60:VAL:N	0.42	2.71	11	2
2:B:145:TYR:O	2:B:145:TYR:CG	0.42	2.70	13	2
1:C:2:LEU:N	1:C:2:LEU:CD1	0.42	2.82	13	1
2:B:114:LEU:CD1	2:B:130:TYR:OH	0.42	2.67	14	1
2:B:100:PRO:C	2:B:102:ASN:HD22	0.42	2.18	15	1
1:C:84:SER:CB	1:C:138:SER:HG	0.42	2.26	16	1
1:A:61:LYS:CG	3:A:142:HEC:HAA2	0.42	2.44	17	1
1:A:113:LEU:HD12	1:A:113:LEU:C	0.42	2.35	18	1
2:B:4:THR:OG1	2:B:7:GLU:OE2	0.42	2.35	19	1
2:B:36:PRO:O	2:B:39:GLN:N	0.42	2.44	19	1
2:D:56:GLY:O	2:D:57:ASN:CG	0.42	2.56	19	1
2:D:26:GLU:OE2	2:D:26:GLU:N	0.42	2.53	20	1
1:C:17:VAL:HG11	1:C:21:ALA:HB2	0.42	1.91	1	1
2:B:42:PHE:CD2	2:B:45:PHE:CD1	0.42	3.07	4	1
1:A:1:VAL:O	1:A:1:VAL:HG12	0.42	2.13	6	1
2:B:97:HIS:ND1	1:C:38:THR:HA	0.42	2.29	7	1
2:D:26:GLU:O	2:D:30:ARG:CG	0.42	2.67	7	1
1:A:9:ASN:C	1:A:124:SER:OG	0.42	2.58	8	1
1:A:34:LEU:C	1:A:34:LEU:CD1	0.42	2.82	9	1
2:B:80:ASN:C	2:B:82:LYS:N	0.42	2.72	10	1
2:B:26:GLU:O	2:B:30:ARG:NH1	0.42	2.52	11	1
2:B:144:LYS:C	2:B:146:HIS:HD1	0.42	2.17	11	1
2:D:17:LYS:N	2:D:17:LYS:HD2	0.42	2.29	15	1
1:A:47:ASP:CG	1:A:54:GLN:HE22	0.42	2.18	17	1
1:C:47:ASP:CG	1:C:54:GLN:HE22	0.42	2.18	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:109:VAL:O	2:B:112:CYS:SG	0.42	2.71	20	1
2:D:105:LEU:HD23	2:D:105:LEU:O	0.42	2.15	20	1
2:D:104:ARG:O	2:D:108:ASN:OD1	0.42	2.37	3	3
1:A:115:ALA:HB1	1:A:121:VAL:CG1	0.42	2.44	5	4
2:B:145:TYR:O	2:B:146:HIS:C	0.42	2.58	5	4
1:C:115:ALA:HB1	1:C:121:VAL:CG1	0.42	2.44	5	4
2:D:119:GLY:C	2:D:121:GLU:N	0.42	2.72	5	1
1:A:50:HIS:O	1:A:50:HIS:ND1	0.42	2.53	6	1
2:B:19:ASN:O	2:B:20:VAL:C	0.42	2.58	10	4
1:A:11:LYS:CD	1:A:11:LYS:N	0.42	2.82	8	1
2:B:50:THR:O	2:B:52:ASP:N	0.42	2.52	9	2
2:D:84:THR:C	2:D:86:ALA:H	0.42	2.18	15	3
2:D:112:CYS:O	2:D:116:HIS:CE1	0.42	2.72	9	1
2:D:114:LEU:HD12	2:D:114:LEU:H	0.42	1.71	9	1
1:A:103:HIS:CB	2:B:108:ASN:ND2	0.42	2.81	10	1
1:C:91:LEU:HD12	1:C:91:LEU:H	0.42	1.74	11	1
2:D:46:GLY:O	2:D:47:ASP:O	0.42	2.37	11	1
1:C:97:ASN:C	1:C:99:LYS:N	0.42	2.73	13	1
1:C:118:THR:O	1:C:118:THR:OG1	0.42	2.36	18	3
1:A:36:PHE:CD2	1:A:100:LEU:HD21	0.42	2.50	15	1
1:A:47:ASP:OD2	1:A:54:GLN:OE1	0.42	2.37	17	1
1:C:61:LYS:CG	3:C:142:HEC:HAA2	0.42	2.44	17	1
1:C:88:ALA:C	1:C:90:LYS:H	0.42	2.16	17	1
1:C:80:LEU:N	1:C:80:LEU:CD1	0.42	2.81	18	1
1:C:93:VAL:CG1	1:C:94:ASP:H	0.42	2.21	18	1
1:C:113:LEU:HD12	1:C:113:LEU:C	0.42	2.35	18	1
1:C:103:HIS:CD2	1:C:103:HIS:O	0.42	2.73	19	1
2:B:63:HIS:NE2	3:B:147:HEC:HHA	0.42	2.24	2	1
2:D:105:LEU:N	2:D:105:LEU:CD2	0.42	2.83	2	1
2:D:106:LEU:CD2	2:D:106:LEU:C	0.42	2.86	3	1
2:D:42:PHE:CD2	2:D:45:PHE:CD1	0.42	3.07	4	1
2:D:80:ASN:OD1	2:D:80:ASN:O	0.42	2.38	8	1
2:D:43:GLU:CD	2:D:44:SER:H	0.42	2.17	9	1
1:A:31:ARG:CG	1:A:31:ARG:HH11	0.42	2.27	12	1
1:C:36:PHE:C	3:C:142:HEC:HMC1	0.42	2.34	12	1
2:D:114:LEU:CD1	2:D:130:TYR:OH	0.42	2.68	14	1
1:C:36:PHE:CD2	1:C:100:LEU:HD21	0.42	2.50	15	1
2:D:39:GLN:OE1	2:D:39:GLN:O	0.42	2.36	16	1
2:B:105:LEU:O	2:B:105:LEU:HD23	0.42	2.15	20	1
2:B:114:LEU:C	2:B:116:HIS:N	0.42	2.71	20	1
1:C:98:PHE:CD1	1:C:99:LYS:N	0.42	2.87	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:45:PHE:O	2:D:46:GLY:O	0.42	2.37	4	1
1:A:127:LYS:HD2	1:A:128:PHE:N	0.42	2.29	7	1
2:B:26:GLU:O	2:B:30:ARG:CG	0.42	2.67	7	1
2:B:17:LYS:H	2:B:17:LYS:HE2	0.42	1.74	8	1
2:B:42:PHE:CZ	2:B:45:PHE:CD2	0.42	3.07	8	1
1:C:2:LEU:HD11	1:C:127:LYS:HE3	0.42	1.91	9	1
2:D:30:ARG:O	2:D:31:LEU:C	0.42	2.58	9	1
2:B:3:LEU:HD13	2:B:8:LYS:HG3	0.42	1.91	10	1
2:D:3:LEU:HD13	2:D:8:LYS:HG3	0.42	1.91	10	1
1:A:97:ASN:C	1:A:99:LYS:N	0.42	2.73	13	1
1:A:48:LEU:C	1:A:50:HIS:H	0.42	2.18	15	1
1:C:47:ASP:OD2	1:C:54:GLN:OE1	0.42	2.37	17	1
1:A:103:HIS:O	1:A:103:HIS:CD2	0.42	2.73	19	1
2:D:100:PRO:O	2:D:102:ASN:OD1	0.42	2.37	19	1
1:A:11:LYS:CD	1:A:11:LYS:H	0.42	2.27	15	2
2:B:106:LEU:HD23	2:B:106:LEU:O	0.42	2.13	3	1
1:C:119:PRO:HA	2:D:33:VAL:HG21	0.42	1.92	3	1
2:D:65:LYS:O	2:D:69:GLY:N	0.42	2.53	3	1
2:B:52:ASP:C	2:B:54:VAL:N	0.42	2.73	4	3
2:B:71:PHE:O	2:B:75:LEU:CD2	0.42	2.68	4	1
2:B:130:TYR:O	2:B:132:LYS:N	0.42	2.53	7	1
1:C:108:THR:O	1:C:109:LEU:C	0.42	2.58	7	1
2:B:106:LEU:HD12	3:B:147:HEC:C1C	0.42	2.41	9	1
1:C:27:GLU:N	1:C:27:GLU:CD	0.42	2.72	9	1
2:D:26:GLU:C	2:D:28:LEU:N	0.42	2.73	14	1
2:D:77:HIS:C	2:D:79:ASP:H	0.42	2.18	18	3
2:B:143:HIS:O	2:B:143:HIS:CG	0.42	2.73	16	1
2:D:143:HIS:O	2:D:143:HIS:CG	0.42	2.73	16	1
1:A:81:SER:O	1:A:85:ASP:OD1	0.42	2.37	17	1
2:B:104:ARG:NH2	2:D:146:HIS:O	0.42	2.53	17	1
1:C:115:ALA:HB2	1:C:122:HIS:CE1	0.42	2.50	17	1
2:D:55:MET:O	2:D:57:ASN:OD1	0.42	2.37	19	1
1:A:11:LYS:NZ	1:A:70:VAL:HG13	0.42	2.29	1	1
2:B:105:LEU:N	2:B:105:LEU:CD2	0.42	2.83	2	1
1:A:94:ASP:OD2	2:D:40:ARG:CZ	0.42	2.68	3	1
2:B:100:PRO:O	2:B:102:ASN:OD1	0.42	2.37	19	2
1:C:94:ASP:C	1:C:96:VAL:H	0.42	2.18	4	2
2:B:139:ASN:O	2:B:142:ALA:N	0.42	2.49	5	1
1:C:50:HIS:O	1:C:50:HIS:ND1	0.42	2.53	6	1
1:A:34:LEU:C	1:A:36:PHE:H	0.42	2.17	12	2
1:C:34:LEU:C	1:C:36:PHE:H	0.42	2.16	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:17:LYS:H	2:D:17:LYS:HE2	0.42	1.74	8	1
1:A:12:ALA:O	1:A:15:GLY:N	0.42	2.51	9	2
2:B:30:ARG:O	2:B:31:LEU:C	0.42	2.58	9	1
1:C:7:LYS:CG	1:C:8:THR:N	0.42	2.83	9	2
2:D:123:THR:C	2:D:127:GLN:HE22	0.42	2.17	11	1
2:B:31:LEU:O	2:B:35:TYR:O	0.42	2.37	12	1
1:C:81:SER:O	1:C:85:ASP:OD1	0.42	2.37	17	2
1:A:86:LEU:HD11	3:A:142:HEC:HBD1	0.42	1.92	15	1
1:C:48:LEU:C	1:C:50:HIS:H	0.42	2.17	15	1
1:C:86:LEU:HD11	3:C:142:HEC:HBD1	0.42	1.92	15	1
1:A:63:ALA:O	1:A:67:THR:OG1	0.42	2.34	17	1
1:A:53:ALA:O	1:A:54:GLN:C	0.42	2.58	19	1
1:C:49:SER:O	1:C:50:HIS:CB	0.42	2.68	19	1
2:D:6:GLU:N	2:D:6:GLU:OE1	0.42	2.52	19	1
2:D:14:LEU:N	2:D:14:LEU:CD1	0.42	2.82	20	1
1:A:95:PRO:O	1:A:96:VAL:C	0.42	2.58	5	4
2:D:52:ASP:C	2:D:54:VAL:N	0.42	2.73	4	5
2:D:81:LEU:O	2:D:84:THR:OG1	0.42	2.37	6	1
2:B:17:LYS:N	2:B:17:LYS:CD	0.42	2.81	18	2
2:D:146:HIS:ND1	2:D:146:HIS:C	0.42	2.71	7	1
2:B:42:PHE:O	2:B:45:PHE:N	0.42	2.48	10	1
1:C:117:PHE:O	1:C:117:PHE:CG	0.42	2.73	10	1
2:D:80:ASN:C	2:D:82:LYS:N	0.42	2.72	10	1
2:D:145:TYR:O	2:D:146:HIS:C	0.42	2.57	16	4
2:D:18:VAL:O	2:D:20:VAL:N	0.42	2.53	12	1
2:D:90:GLU:O	2:D:94:ASP:N	0.42	2.45	16	2
1:C:3:SER:OG	1:C:6:ASP:OD1	0.42	2.37	16	1
1:A:115:ALA:HB2	1:A:122:HIS:CE1	0.42	2.50	17	1
1:A:2:LEU:C	1:A:3:SER:OG	0.42	2.57	18	1
1:A:92:ARG:NE	2:D:40:ARG:HD2	0.42	2.20	18	1
1:A:129:LEU:O	1:A:133:SER:CB	0.42	2.67	18	1
1:C:129:LEU:O	1:C:133:SER:CB	0.42	2.67	18	1
1:C:110:ALA:O	1:C:112:HIS:N	0.41	2.53	1	1
2:D:71:PHE:CE2	2:D:134:VAL:HG11	0.41	2.50	3	1
2:B:2:HIS:O	2:B:2:HIS:CG	0.41	2.72	4	1
1:C:31:ARG:O	1:C:35:SER:OG	0.41	2.37	4	1
1:C:109:LEU:O	1:C:113:LEU:N	0.41	2.53	14	6
1:C:127:LYS:CD	1:C:127:LYS:C	0.41	2.88	5	2
2:B:81:LEU:O	2:B:84:THR:OG1	0.41	2.37	6	1
2:D:87:THR:OG1	2:D:88:LEU:N	0.41	2.53	6	1
1:A:7:LYS:CG	1:A:8:THR:N	0.41	2.83	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:101:LEU:HD23	3:C:142:HEC:HBB3	0.41	1.91	14	1
2:D:40:ARG:C	2:D:42:PHE:H	0.41	2.17	15	1
2:B:37:TRP:CG	2:B:38:THR:N	0.41	2.88	16	1
1:A:63:ALA:O	1:A:67:THR:CB	0.41	2.68	17	1
2:B:26:GLU:N	2:B:26:GLU:OE2	0.41	2.52	20	1
1:C:7:LYS:O	1:C:8:THR:C	0.41	2.58	15	5
1:C:21:ALA:C	1:C:23:GLU:H	0.41	2.19	10	5
1:C:86:LEU:HD21	3:C:142:HEC:CGD	0.41	2.45	7	1
2:B:30:ARG:O	2:B:34:VAL:HG22	0.41	2.15	8	1
2:D:30:ARG:O	2:D:34:VAL:HG22	0.41	2.15	8	1
1:A:3:SER:H	1:A:4:PRO:CD	0.41	2.28	10	1
2:B:6:GLU:N	2:B:6:GLU:CD	0.41	2.73	10	1
1:C:50:HIS:CG	1:C:51:GLY:H	0.41	2.33	11	1
1:A:47:ASP:O	1:A:52:SER:CB	0.41	2.69	13	1
2:D:52:ASP:OD1	2:D:53:ALA:N	0.41	2.53	13	1
2:B:102:ASN:ND2	3:B:147:HEC:CMC	0.41	2.83	14	1
1:C:32:MET:O	1:C:33:PHE:C	0.41	2.59	18	2
2:B:68:LEU:HD23	2:B:68:LEU:O	0.41	2.16	17	1
1:C:50:HIS:C	1:C:52:SER:N	0.41	2.73	17	1
2:B:103:PHE:C	2:B:105:LEU:N	0.41	2.74	1	1
2:D:20:VAL:C	2:D:22:GLU:H	0.41	2.18	15	2
2:D:71:PHE:O	2:D:75:LEU:CD2	0.41	2.68	4	1
2:D:93:CYS:O	2:D:97:HIS:CG	0.41	2.74	7	1
2:D:130:TYR:O	2:D:132:LYS:N	0.41	2.53	7	1
1:A:11:LYS:N	1:A:11:LYS:HD2	0.41	2.31	8	1
1:A:103:HIS:HB3	2:B:108:ASN:ND2	0.41	2.30	10	1
3:A:142:HEC:HBB3	3:A:142:HEC:CMB	0.41	2.40	12	1
1:C:47:ASP:O	1:C:52:SER:CB	0.41	2.69	13	1
1:C:61:LYS:HB3	3:C:142:HEC:CMA	0.41	2.44	17	2
2:B:55:MET:O	2:B:57:ASN:OD1	0.41	2.37	19	1
2:D:22:GLU:O	2:D:23:VAL:C	0.41	2.59	20	1
2:D:19:ASN:O	2:D:20:VAL:C	0.41	2.59	9	5
1:A:29:LEU:O	1:A:30:GLU:C	0.41	2.58	3	1
2:B:14:LEU:HD23	2:B:17:LYS:HD3	0.41	1.92	3	1
2:B:146:HIS:HB3	2:D:135:ALA:HB3	0.41	1.91	3	1
1:A:64:ASP:O	1:A:68:ASN:N	0.41	2.41	4	1
1:A:109:LEU:O	1:A:113:LEU:N	0.41	2.53	17	6
2:D:92:HIS:O	2:D:145:TYR:OH	0.41	2.35	6	1
2:B:30:ARG:HH21	2:B:33:VAL:HG11	0.41	1.75	7	1
2:D:131:GLN:O	2:D:135:ALA:N	0.41	2.49	9	1
1:A:134:THR:O	1:A:138:SER:CB	0.41	2.69	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:71:PHE:O	2:D:74:GLY:N	0.41	2.50	12	1
2:B:139:ASN:O	2:B:139:ASN:ND2	0.41	2.52	15	1
1:A:84:SER:OG	1:A:136:LEU:O	0.41	2.37	16	1
1:C:84:SER:OG	1:C:136:LEU:O	0.41	2.36	20	2
1:A:88:ALA:C	1:A:90:LYS:N	0.41	2.73	17	1
2:D:68:LEU:HD23	2:D:68:LEU:O	0.41	2.16	17	1
2:B:14:LEU:N	2:B:14:LEU:CD1	0.41	2.82	20	1
2:D:103:PHE:C	2:D:105:LEU:N	0.41	2.74	1	1
1:A:101:LEU:HD23	3:A:142:HEC:HBB3	0.41	1.91	14	2
2:B:135:ALA:HB1	2:D:146:HIS:ND1	0.41	2.30	3	1
1:C:95:PRO:O	1:C:96:VAL:C	0.41	2.58	5	2
2:B:131:GLN:CD	2:B:131:GLN:N	0.41	2.74	5	2
1:C:101:LEU:CD1	3:C:142:HEC:HMC3	0.41	2.34	7	1
1:A:62:VAL:HG22	3:A:142:HEC:C2B	0.41	2.45	8	1
2:B:17:LYS:H	2:B:17:LYS:HD2	0.41	1.74	8	1
2:D:104:ARG:NH1	2:D:104:ARG:CB	0.41	2.84	12	1
1:C:126:ASP:CG	2:D:35:TYR:CD2	0.41	2.93	13	1
2:D:96:LEU:O	2:D:98:VAL:N	0.41	2.54	13	1
2:B:47:ASP:OD1	2:B:47:ASP:N	0.41	2.47	16	1
2:B:97:HIS:O	2:B:98:VAL:C	0.41	2.59	16	1
2:D:37:TRP:CG	2:D:38:THR:N	0.41	2.89	16	1
1:C:63:ALA:O	1:C:67:THR:CB	0.41	2.68	17	1
1:A:32:MET:O	1:A:35:SER:N	0.41	2.53	18	1
1:C:100:LEU:C	1:C:102:SER:N	0.41	2.72	20	1
2:D:84:THR:C	2:D:86:ALA:N	0.41	2.73	20	1
2:B:45:PHE:C	2:B:47:ASP:H	0.41	2.18	5	1
2:D:37:TRP:CE2	2:D:38:THR:HG23	0.41	2.51	6	2
2:D:41:PHE:CD1	2:D:41:PHE:N	0.41	2.89	6	1
1:A:21:ALA:C	1:A:23:GLU:H	0.41	2.19	10	4
1:A:2:LEU:HD11	1:A:127:LYS:HE3	0.41	1.92	9	1
2:B:46:GLY:O	2:B:47:ASP:O	0.41	2.37	11	1
2:D:144:LYS:C	2:D:146:HIS:HD1	0.41	2.17	11	1
1:A:2:LEU:N	1:A:2:LEU:CD1	0.41	2.83	13	1
2:B:52:ASP:OD1	2:B:53:ALA:N	0.41	2.53	13	1
1:C:97:ASN:O	1:C:99:LYS:N	0.41	2.54	13	1
2:B:84:THR:C	2:B:86:ALA:H	0.41	2.18	15	2
3:B:147:HEC:CMC	2:D:31:LEU:CD2	0.41	2.99	15	1
1:A:17:VAL:HG13	1:A:24:TYR:CD2	0.41	2.50	16	1
1:C:18:GLY:C	1:C:20:HIS:N	0.41	2.74	16	1
1:A:19:ALA:O	1:A:20:HIS:CG	0.41	2.73	17	1
1:A:75:ASP:OD2	1:A:78:ASN:OD1	0.41	2.38	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ASN:CB	3:A:142:HEC:CMC	0.41	2.97	17	1
2:D:38:THR:O	2:D:41:PHE:N	0.41	2.46	19	1
1:C:106:LEU:CD1	1:C:122:HIS:CE1	0.41	2.99	4	1
2:D:8:LYS:O	2:D:9:SER:C	0.41	2.59	4	1
1:A:86:LEU:HD21	3:A:142:HEC:CGD	0.41	2.45	7	1
2:D:42:PHE:C	2:D:44:SER:H	0.41	2.19	7	1
1:A:2:LEU:HD21	1:A:6:ASP:OD1	0.41	2.16	9	1
1:A:17:VAL:HG13	1:A:24:TYR:CE2	0.41	2.51	12	1
2:D:133:VAL:O	2:D:134:VAL:C	0.41	2.59	12	1
2:D:77:HIS:O	2:D:79:ASP:N	0.41	2.54	14	1
2:B:121:GLU:C	2:B:123:THR:H	0.41	2.18	15	1
1:C:65:ALA:HB3	3:C:142:HEC:HMB3	0.41	1.90	20	1
1:A:110:ALA:O	1:A:112:HIS:N	0.41	2.53	1	1
1:C:47:ASP:OD1	1:C:47:ASP:O	0.41	2.37	2	1
1:C:117:PHE:CE1	2:D:116:HIS:CE1	0.41	3.07	4	1
1:C:46:PHE:CE2	1:C:55:VAL:HG22	0.41	2.51	5	1
2:D:45:PHE:C	2:D:47:ASP:H	0.41	2.18	5	1
1:A:83:LEU:N	1:A:83:LEU:HD23	0.41	2.31	11	3
1:C:62:VAL:HG22	3:C:142:HEC:C2B	0.41	2.45	8	1
2:D:67:VAL:HG13	3:D:147:HEC:HMB3	0.41	1.91	9	1
1:C:134:THR:O	1:C:138:SER:CB	0.41	2.69	10	1
2:B:66:LYS:O	3:B:147:HEC:HMA3	0.41	2.15	12	1
2:B:37:TRP:C	2:B:39:GLN:H	0.41	2.17	14	1
1:A:32:MET:O	1:A:33:PHE:C	0.41	2.59	16	1
2:B:73:ASP:O	2:B:77:HIS:N	0.41	2.53	17	1
1:A:92:ARG:HB3	2:D:40:ARG:HE	0.41	1.73	18	1
2:B:8:LYS:C	2:B:10:ALA:N	0.41	2.74	19	1
2:B:22:GLU:O	2:B:23:VAL:C	0.41	2.59	20	1
2:B:26:GLU:N	2:B:26:GLU:CD	0.41	2.74	20	1
1:C:3:SER:OG	1:C:4:PRO:CD	0.41	2.69	20	1
1:A:78:ASN:HD22	1:A:78:ASN:C	0.41	2.18	2	1
1:C:3:SER:H	1:C:4:PRO:CD	0.41	2.29	2	1
1:A:46:PHE:CE2	1:A:55:VAL:HG22	0.41	2.51	5	2
2:B:71:PHE:CE2	2:B:134:VAL:HG11	0.41	2.50	3	1
1:A:94:ASP:C	1:A:96:VAL:H	0.41	2.18	4	2
2:B:37:TRP:CE2	2:B:38:THR:HG23	0.41	2.51	6	2
2:D:44:SER:C	2:D:46:GLY:H	0.41	2.19	6	1
1:A:98:PHE:CE1	1:A:133:SER:CB	0.41	3.04	7	1
2:B:93:CYS:O	2:B:97:HIS:CG	0.41	2.74	7	1
1:C:24:TYR:CD1	1:C:112:HIS:CE1	0.41	3.09	7	1
1:C:48:LEU:C	1:C:48:LEU:CD2	0.41	2.90	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:120:ALA:O	1:C:121:VAL:C	0.41	2.59	9	1
1:A:27:GLU:OE2	1:A:112:HIS:CD2	0.41	2.74	10	1
1:A:37:PRO:O	1:A:38:THR:C	0.41	2.59	10	1
2:B:97:HIS:CE1	1:C:94:ASP:OD2	0.41	2.74	10	1
1:C:103:HIS:HB3	2:D:108:ASN:ND2	0.41	2.30	10	1
2:D:21:ASP:C	2:D:65:LYS:NZ	0.41	2.74	10	1
2:B:99:ASP:CB	1:C:96:VAL:HG11	0.41	2.41	11	1
2:B:97:HIS:NE2	1:C:41:THR:CB	0.41	2.84	12	1
2:B:133:VAL:O	2:B:134:VAL:C	0.41	2.59	12	1
2:B:13:ALA:O	2:B:16:GLY:N	0.41	2.52	14	1
1:C:86:LEU:HD11	3:C:142:HEC:O1D	0.41	2.16	14	1
2:D:37:TRP:O	2:D:39:GLN:N	0.41	2.51	14	1
2:D:102:ASN:ND2	3:D:147:HEC:CMC	0.41	2.83	14	1
1:A:75:ASP:C	1:A:77:PRO:HD2	0.41	2.37	15	1
3:B:147:HEC:CHB	2:D:67:VAL:HA	0.41	2.46	15	1
1:A:31:ARG:NH2	1:A:34:LEU:CD1	0.41	2.84	16	1
1:A:4:PRO:O	1:A:5:ALA:C	0.41	2.60	17	1
1:A:117:PHE:CD2	1:A:117:PHE:O	0.41	2.74	17	1
1:C:75:ASP:OD2	1:C:78:ASN:OD1	0.41	2.38	17	1
1:C:117:PHE:CD2	1:C:117:PHE:O	0.41	2.74	17	1
1:A:92:ARG:HD2	2:D:40:ARG:NH1	0.41	2.31	18	1
2:B:106:LEU:HD13	2:B:106:LEU:O	0.41	2.15	18	1
1:C:32:MET:O	1:C:35:SER:N	0.41	2.53	18	1
2:B:134:VAL:C	2:B:136:GLY:N	0.41	2.73	19	1
1:A:3:SER:OG	1:A:4:PRO:CD	0.41	2.69	20	1
2:D:14:LEU:CD1	2:D:14:LEU:H	0.41	2.29	20	1
1:A:90:LYS:O	1:A:91:LEU:CB	0.41	2.67	1	1
2:B:41:PHE:C	2:B:43:GLU:H	0.41	2.19	3	1
2:B:52:ASP:O	2:B:54:VAL:N	0.41	2.54	14	3
1:A:1:VAL:C	1:A:2:LEU:HD12	0.41	2.37	5	1
2:D:131:GLN:CD	2:D:131:GLN:N	0.41	2.74	5	2
1:A:125:LEU:O	1:A:129:LEU:HB3	0.41	2.16	7	1
2:D:30:ARG:HH21	2:D:33:VAL:HG11	0.41	1.76	7	1
1:C:83:LEU:N	1:C:83:LEU:HD23	0.41	2.31	11	1
2:B:96:LEU:O	2:B:98:VAL:N	0.41	2.54	13	1
1:C:13:ALA:O	1:C:17:VAL:CG2	0.41	2.68	13	1
1:A:86:LEU:HD11	3:A:142:HEC:O1D	0.41	2.16	14	1
1:A:115:ALA:O	1:A:117:PHE:N	0.41	2.53	15	1
1:A:38:THR:O	1:A:39:THR:C	0.41	2.59	16	1
1:C:38:THR:O	1:C:39:THR:C	0.41	2.59	16	1
1:C:4:PRO:O	1:C:5:ALA:C	0.41	2.60	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:19:ALA:O	1:C:20:HIS:CG	0.41	2.73	17	1
1:C:23:GLU:O	1:C:26:ALA:HB3	0.41	2.16	17	1
1:C:88:ALA:C	1:C:90:LYS:N	0.41	2.73	17	1
1:A:50:HIS:CD2	1:A:50:HIS:N	0.41	2.88	18	1
2:B:88:LEU:O	2:B:92:HIS:CG	0.41	2.74	18	1
2:B:105:LEU:C	2:B:107:GLY:N	0.40	2.75	1	1
2:D:116:HIS:C	2:D:116:HIS:ND1	0.40	2.75	1	1
2:D:83:GLY:O	2:D:86:ALA:N	0.40	2.43	4	1
2:D:89:SER:OG	2:D:140:ALA:O	0.40	2.37	5	1
2:B:41:PHE:CD1	2:B:41:PHE:N	0.40	2.90	7	2
2:B:87:THR:OG1	2:B:88:LEU:N	0.40	2.53	6	1
1:A:4:PRO:C	1:A:6:ASP:H	0.40	2.20	7	1
2:B:42:PHE:C	2:B:44:SER:H	0.40	2.20	7	1
1:A:109:LEU:HD23	1:A:109:LEU:H	0.40	1.75	12	1
1:C:10:VAL:HG21	1:C:128:PHE:CD1	0.40	2.51	13	1
1:C:116:GLU:O	1:C:117:PHE:C	0.40	2.60	14	1
1:C:17:VAL:HG13	1:C:24:TYR:CD2	0.40	2.50	16	1
1:A:2:LEU:CD2	1:A:131:SER:OG	0.40	2.68	19	1
2:B:106:LEU:HD22	3:B:147:HEC:HBB3	0.40	0.43	19	1
2:B:2:HIS:ND1	2:B:2:HIS:C	0.40	2.74	3	1
2:B:59:LYS:CG	2:B:60:VAL:N	0.40	2.85	6	1
1:C:80:LEU:C	1:C:82:ALA:N	0.40	2.75	8	1
2:B:21:ASP:C	2:B:65:LYS:NZ	0.40	2.74	10	1
1:A:38:THR:C	1:A:40:LYS:N	0.40	2.75	11	1
1:A:30:GLU:OE2	1:A:30:GLU:O	0.40	2.40	12	1
1:C:17:VAL:HG13	1:C:24:TYR:CE2	0.40	2.51	12	1
1:A:77:PRO:O	1:A:81:SER:OG	0.40	2.35	13	1
1:A:96:VAL:HG21	2:D:99:ASP:OD1	0.40	2.15	13	1
2:B:95:LYS:O	2:B:96:LEU:HD12	0.40	2.17	13	1
1:C:76:MET:SD	1:C:132:VAL:HG22	0.40	2.56	13	1
1:A:7:LYS:NZ	1:A:7:LYS:CB	0.40	2.84	14	1
2:B:26:GLU:C	2:B:28:LEU:N	0.40	2.73	14	1
1:C:115:ALA:O	1:C:117:PHE:N	0.40	2.53	15	1
2:D:139:ASN:O	2:D:139:ASN:ND2	0.40	2.52	15	1
1:A:18:GLY:C	1:A:20:HIS:N	0.40	2.74	16	1
1:C:31:ARG:NH2	1:C:34:LEU:CD1	0.40	2.84	16	1
1:C:126:ASP:OD2	2:D:35:TYR:CZ	0.40	2.75	17	1
2:B:8:LYS:O	2:B:9:SER:C	0.40	2.59	18	1
2:D:106:LEU:HD13	2:D:106:LEU:O	0.40	2.15	18	1
2:B:38:THR:O	2:B:41:PHE:N	0.40	2.46	19	1
2:D:134:VAL:C	2:D:136:GLY:N	0.40	2.73	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:47:ASP:CG	2:B:48:LEU:H	0.40	2.19	20	1
2:B:105:LEU:N	2:B:105:LEU:HD22	0.40	2.32	2	1
2:D:90:GLU:HA	2:D:144:LYS:HZ2	0.40	1.77	2	1
2:D:48:LEU:O	2:D:49:SER:C	0.40	2.60	3	2
2:B:44:SER:C	2:B:46:GLY:H	0.40	2.19	6	1
2:B:59:LYS:O	2:B:60:VAL:C	0.40	2.59	7	1
1:C:98:PHE:CE1	1:C:133:SER:CB	0.40	3.04	7	1
2:B:97:HIS:CE1	1:C:41:THR:OG1	0.40	2.74	12	1
2:B:104:ARG:NH1	2:B:104:ARG:CB	0.40	2.84	12	1
1:A:126:ASP:CG	2:B:35:TYR:CD2	0.40	2.93	13	1
2:D:95:LYS:O	2:D:96:LEU:HD12	0.40	2.17	13	1
1:A:121:VAL:HG12	1:A:122:HIS:N	0.40	2.31	15	1
1:C:47:ASP:O	1:C:48:LEU:C	0.40	2.59	19	1
2:D:8:LYS:C	2:D:10:ALA:N	0.40	2.74	19	1
1:A:65:ALA:CB	3:A:142:HEC:CMB	0.40	2.99	20	1
1:C:33:PHE:O	1:C:34:LEU:C	0.40	2.59	3	1
1:A:104:CYS:O	1:A:107:VAL:N	0.40	2.54	5	1
1:C:1:VAL:C	1:C:2:LEU:HD12	0.40	2.37	5	1
1:A:80:LEU:C	1:A:82:ALA:N	0.40	2.75	8	1
1:C:2:LEU:HD21	1:C:6:ASP:OD1	0.40	2.16	9	1
1:A:99:LYS:O	1:A:103:HIS:CE1	0.40	2.75	10	1
1:A:117:PHE:O	1:A:117:PHE:CG	0.40	2.73	10	1
1:C:109:LEU:HD23	1:C:109:LEU:H	0.40	1.75	12	1
2:D:122:PHE:O	2:D:123:THR:C	0.40	2.60	16	1
1:A:50:HIS:C	1:A:52:SER:N	0.40	2.73	17	1
1:A:107:VAL:HG11	2:B:127:GLN:NE2	0.40	2.29	17	1
1:A:119:PRO:CA	2:B:33:VAL:HG13	0.40	2.46	17	1
2:D:73:ASP:O	2:D:77:HIS:N	0.40	2.53	17	1
1:A:29:LEU:CD1	1:A:58:HIS:CG	0.40	3.05	18	1
1:A:93:VAL:HG13	1:A:93:VAL:O	0.40	2.17	19	1
1:C:2:LEU:CD2	1:C:131:SER:OG	0.40	2.68	19	1
1:C:131:SER:O	1:C:135:VAL:CG2	0.40	2.70	19	1
2:D:126:VAL:HG12	2:D:126:VAL:O	0.40	2.16	19	1
1:A:119:PRO:HA	2:B:33:VAL:HG21	0.40	1.92	3	1
2:B:97:HIS:ND1	1:C:41:THR:HB	0.40	2.32	4	1
1:A:24:TYR:CD1	1:A:112:HIS:CE1	0.40	3.09	7	1
1:A:113:LEU:O	1:A:113:LEU:HD23	0.40	2.17	10	1
1:C:99:LYS:O	1:C:103:HIS:CE1	0.40	2.75	10	1
1:C:113:LEU:O	1:C:113:LEU:HD23	0.40	2.17	10	1
1:A:48:LEU:C	1:A:48:LEU:CD2	0.40	2.90	11	1
1:A:50:HIS:CG	1:A:51:GLY:H	0.40	2.33	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:18:VAL:O	2:B:20:VAL:N	0.40	2.53	12	1
2:B:79:ASP:O	2:B:80:ASN:CG	0.40	2.60	13	1
2:B:77:HIS:O	2:B:79:ASP:N	0.40	2.54	14	1
2:B:122:PHE:O	2:B:123:THR:C	0.40	2.60	16	1
2:D:97:HIS:O	2:D:98:VAL:C	0.40	2.59	16	1
2:B:146:HIS:C	2:D:104:ARG:NH2	0.40	2.74	17	1
1:C:119:PRO:CA	2:D:33:VAL:HG13	0.40	2.46	17	1
2:D:88:LEU:O	2:D:92:HIS:CG	0.40	2.74	18	1
2:B:84:THR:C	2:B:86:ALA:N	0.40	2.73	20	1
2:D:26:GLU:N	2:D:26:GLU:CD	0.40	2.74	20	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	134/141 (95%)	100±3 (74±2%)	22±3 (16±2%)	13±2 (9±2%)	1	11
1	C	134/141 (95%)	100±3 (74±2%)	22±3 (16±2%)	13±2 (9±2%)	1	11
2	B	144/146 (99%)	111±4 (77±3%)	29±4 (20±3%)	4±2 (3±1%)	7	40
2	D	144/146 (99%)	111±4 (77±3%)	29±4 (20±3%)	4±2 (3±1%)	7	40
All	All	11120/11480 (97%)	8418 (76%)	2024 (18%)	678 (6%)	3	20

All 118 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	73	VAL	20
1	C	73	VAL	20
1	A	75	ASP	19
1	A	119	PRO	19
1	C	75	ASP	19
1	C	119	PRO	19
1	A	19	ALA	17
1	C	19	ALA	17

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Mol	Chain	Res	Type	Models (Total)
1	A	47	ASP	16
1	A	114	PRO	16
1	C	47	ASP	16
1	C	114	PRO	16
1	A	4	PRO	15
1	C	4	PRO	15
2	B	20	VAL	12
2	B	77	HIS	12
2	D	20	VAL	12
2	D	77	HIS	12
1	A	3	SER	11
1	A	116	GLU	11
1	C	3	SER	11
1	C	116	GLU	11
1	A	90	LYS	10
1	C	90	LYS	10
1	A	45	HIS	8
1	A	95	PRO	8
1	C	45	HIS	8
1	C	95	PRO	8
1	A	53	ALA	7
2	B	2	HIS	7
1	C	53	ALA	7
2	D	2	HIS	7
1	A	96	VAL	7
1	A	138	SER	7
2	B	102	ASN	7
1	C	96	VAL	7
1	C	138	SER	7
2	D	102	ASN	7
1	A	50	HIS	6
1	A	93	VAL	6
1	C	50	HIS	6
1	C	93	VAL	6
2	B	47	ASP	6
2	B	100	PRO	6
2	D	47	ASP	6
2	D	100	PRO	6
1	A	2	LEU	5
1	C	2	LEU	5
1	A	52	SER	5
1	C	52	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	A	5	ALA	5
1	C	5	ALA	5
2	B	58	PRO	5
2	D	58	PRO	5
1	A	6	ASP	4
2	B	46	GLY	4
1	C	6	ASP	4
2	D	46	GLY	4
1	A	54	GLN	4
1	C	54	GLN	4
1	A	92	ARG	4
2	B	38	THR	4
1	C	92	ARG	4
2	D	38	THR	4
1	A	88	ALA	4
1	C	88	ALA	4
2	B	80	ASN	3
2	D	80	ASN	3
1	A	48	LEU	3
1	C	48	LEU	3
1	A	91	LEU	3
1	C	91	LEU	3
1	A	18	GLY	3
1	C	18	GLY	3
1	A	37	PRO	2
1	C	37	PRO	2
2	B	15	TRP	2
2	B	39	GLN	2
2	B	43	GLU	2
2	D	15	TRP	2
2	D	39	GLN	2
2	D	43	GLU	2
1	A	38	THR	2
1	C	38	THR	2
2	B	14	LEU	2
2	D	14	LEU	2
2	B	145	TYR	2
2	D	145	TYR	2
1	A	41	THR	2
1	C	41	THR	2
2	B	42	PHE	1
2	D	42	PHE	1

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Mol	Chain	Res	Type	Models (Total)
2	B	97	HIS	1
2	D	97	HIS	1
1	A	35	SER	1
1	C	35	SER	1
1	A	94	ASP	1
1	C	94	ASP	1
2	B	101	GLU	1
2	D	101	GLU	1
2	B	134	VAL	1
2	D	134	VAL	1
2	B	5	PRO	1
2	D	5	PRO	1
1	A	120	ALA	1
2	B	37	TRP	1
2	B	122	PHE	1
1	C	120	ALA	1
2	D	37	TRP	1
2	D	122	PHE	1
1	A	33	PHE	1
1	C	33	PHE	1
2	B	57	ASN	1
2	B	108	ASN	1
2	D	57	ASN	1
2	D	108	ASN	1
2	B	40	ARG	1
2	D	40	ARG	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/113 (95%)	94±3 (88±2%)	13±3 (12±2%)	8	51
1	C	107/113 (95%)	94±3 (88±2%)	13±3 (12±2%)	8	51
2	B	117/118 (99%)	104±2 (89±2%)	13±2 (11±2%)	9	53
2	D	117/118 (99%)	104±2 (89±2%)	13±2 (11±2%)	9	53
All	All	8960/9240 (97%)	7927 (88%)	1033 (12%)	9	52

All 224 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	3	SER	20
1	A	127	LYS	20
1	C	3	SER	20
1	C	127	LYS	20
1	A	14	TRP	19
1	C	14	TRP	19
2	B	3	LEU	18
2	B	122	PHE	18
2	D	3	LEU	18
2	D	122	PHE	18
1	A	61	LYS	15
1	A	113	LEU	15
1	C	61	LYS	15
1	C	113	LEU	15
2	B	17	LYS	14
2	D	17	LYS	14
2	B	14	LEU	13
2	D	14	LEU	13
1	A	46	PHE	12
1	A	136	LEU	12
2	B	95	LYS	12
2	B	116	HIS	12
1	C	46	PHE	12
1	C	136	LEU	12
2	D	95	LYS	12
2	D	116	HIS	12
2	B	8	LYS	11
2	D	8	LYS	11
1	A	118	THR	11
1	C	118	THR	11
1	A	48	LEU	10
2	B	15	TRP	10
1	C	48	LEU	10
2	D	15	TRP	10
1	A	31	ARG	9
1	A	45	HIS	9
1	C	31	ARG	9
1	C	45	HIS	9
2	B	34	VAL	8
2	D	34	VAL	8
2	B	99	ASP	8

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Mol	Chain	Res	Type	Models (Total)
2	D	99	ASP	8
1	A	11	LYS	7
1	C	11	LYS	7
2	B	96	LEU	7
2	D	96	LEU	7
2	B	59	LYS	7
2	B	145	TYR	7
2	D	59	LYS	7
2	D	145	TYR	7
2	B	144	LYS	6
2	D	144	LYS	6
1	A	105	LEU	6
1	A	122	HIS	6
2	B	4	THR	6
1	C	105	LEU	6
1	C	122	HIS	6
2	D	4	THR	6
1	A	94	ASP	6
1	C	94	ASP	6
2	B	146	HIS	6
2	D	146	HIS	6
1	A	41	THR	5
2	B	84	THR	5
1	C	41	THR	5
2	D	84	THR	5
1	A	98	PHE	5
1	C	98	PHE	5
2	B	37	TRP	5
2	D	37	TRP	5
2	B	97	HIS	5
2	D	97	HIS	5
1	A	78	ASN	4
2	B	55	MET	4
2	B	130	TYR	4
1	C	78	ASN	4
2	D	55	MET	4
2	D	130	TYR	4
2	B	2	HIS	4
2	B	127	GLN	4
2	D	2	HIS	4
2	D	127	GLN	4
2	B	11	VAL	4

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Mol	Chain	Res	Type	Models (Total)
2	D	11	VAL	4
1	A	33	PHE	4
1	C	33	PHE	4
1	A	7	LYS	4
1	C	7	LYS	4
2	B	102	ASN	4
2	D	102	ASN	4
1	A	50	HIS	3
1	A	56	LYS	3
2	B	123	THR	3
1	C	50	HIS	3
1	C	56	LYS	3
2	D	123	THR	3
2	B	80	ASN	3
2	D	80	ASN	3
2	B	35	TYR	3
2	D	35	TYR	3
1	A	75	ASP	3
1	C	75	ASP	3
1	A	76	MET	3
1	C	76	MET	3
2	B	30	ARG	3
2	D	30	ARG	3
1	A	58	HIS	3
1	A	97	ASN	3
1	C	58	HIS	3
1	C	66	LEU	3
1	C	97	ASN	3
2	B	65	LYS	3
2	D	65	LYS	3
2	B	117	HIS	3
2	D	117	HIS	3
1	A	36	PHE	2
2	B	61	LYS	2
2	B	103	PHE	2
1	C	36	PHE	2
2	D	61	LYS	2
2	D	103	PHE	2
2	B	21	ASP	2
2	B	48	LEU	2
2	B	94	ASP	2
2	D	21	ASP	2

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Mol	Chain	Res	Type	Models (Total)
2	D	48	LEU	2
2	D	94	ASP	2
2	B	50	THR	2
2	D	50	THR	2
1	A	131	SER	2
2	B	133	VAL	2
1	C	131	SER	2
2	D	133	VAL	2
1	A	90	LYS	2
2	B	57	ASN	2
1	C	90	LYS	2
2	D	57	ASN	2
1	A	99	LYS	2
1	A	129	LEU	2
1	C	99	LYS	2
1	C	129	LEU	2
1	A	32	MET	2
1	A	81	SER	2
2	B	82	LYS	2
2	B	108	ASN	2
1	C	32	MET	2
1	C	81	SER	2
2	D	82	LYS	2
2	D	108	ASN	2
1	A	66	LEU	2
2	B	52	ASP	2
2	D	52	ASP	2
1	A	89	HIS	2
1	C	89	HIS	2
1	A	109	LEU	2
1	C	109	LEU	2
2	B	139	ASN	2
2	D	139	ASN	2
2	B	63	HIS	2
2	D	63	HIS	2
2	B	7	GLU	2
2	D	7	GLU	2
1	A	91	LEU	1
1	A	108	THR	1
1	C	91	LEU	1
1	C	108	THR	1
2	B	47	ASP	1

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Mol	Chain	Res	Type	Models (Total)
2	B	71	PHE	1
2	D	47	ASP	1
2	D	71	PHE	1
1	A	116	GLU	1
2	B	9	SER	1
2	B	42	PHE	1
2	B	66	LYS	1
1	C	116	GLU	1
2	D	9	SER	1
2	D	42	PHE	1
2	D	66	LYS	1
2	B	114	LEU	1
2	D	114	LEU	1
1	A	112	HIS	1
1	A	124	SER	1
1	C	112	HIS	1
1	C	124	SER	1
1	A	1	VAL	1
1	A	83	LEU	1
1	A	103	HIS	1
1	C	1	VAL	1
1	C	83	LEU	1
1	C	103	HIS	1
1	A	84	SER	1
1	C	84	SER	1
2	B	39	GLN	1
2	B	43	GLU	1
2	D	39	GLN	1
2	D	43	GLU	1
1	A	135	VAL	1
1	C	135	VAL	1
2	B	19	ASN	1
2	D	19	ASN	1
1	A	30	GLU	1
1	C	30	GLU	1
1	A	54	GLN	1
1	C	54	GLN	1
1	A	47	ASP	1
1	A	49	SER	1
1	A	93	VAL	1
2	B	28	LEU	1
2	B	72	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	C	47	ASP	1
1	C	49	SER	1
1	C	93	VAL	1
2	D	28	LEU	1
2	D	72	SER	1
1	A	27	GLU	1
1	A	138	SER	1
1	C	27	GLU	1
1	C	138	SER	1
1	A	85	ASP	1
1	C	85	ASP	1
1	A	40	LYS	1
1	C	40	LYS	1
2	B	92	HIS	1
2	D	92	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	HEC	C	142	-	26,50,50	1.68±0.03	2±0 (7±0%)
3	HEC	B	147	-	26,50,50	1.67±0.02	2±0 (7±0%)
3	HEC	A	142	-	26,50,50	1.68±0.02	2±0 (7±0%)
3	HEC	D	147	-	26,50,50	1.67±0.02	2±0 (7±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	HEC	C	142	-	18,82,82	0.89±0.02	0±0 (0±0%)
3	HEC	B	147	-	18,82,82	0.92±0.01	0±0 (0±0%)
3	HEC	A	142	-	18,82,82	0.89±0.02	0±0 (0±0%)
3	HEC	D	147	-	18,82,82	0.92±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	147	-	-	0±0,6,54,54	-
3	HEC	C	142	-	-	0±0,6,54,54	-
3	HEC	A	142	-	-	0±0,6,54,54	-
3	HEC	D	147	-	-	0±0,6,54,54	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	142	HEC	C2B-C3B	5.24	1.35	1.40	5	20
3	C	142	HEC	C2B-C3B	5.21	1.35	1.40	18	20
3	B	147	HEC	C2B-C3B	5.16	1.35	1.40	18	20
3	D	147	HEC	C3C-C2C	5.15	1.35	1.40	14	20
3	D	147	HEC	C2B-C3B	5.13	1.35	1.40	18	20
3	A	142	HEC	C3C-C2C	5.05	1.35	1.40	20	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	147	HEC	C3C-C2C	5.04	1.35	1.40	1	20
3	C	142	HEC	C3C-C2C	5.04	1.35	1.40	19	20

There are no bond-angle outliers.

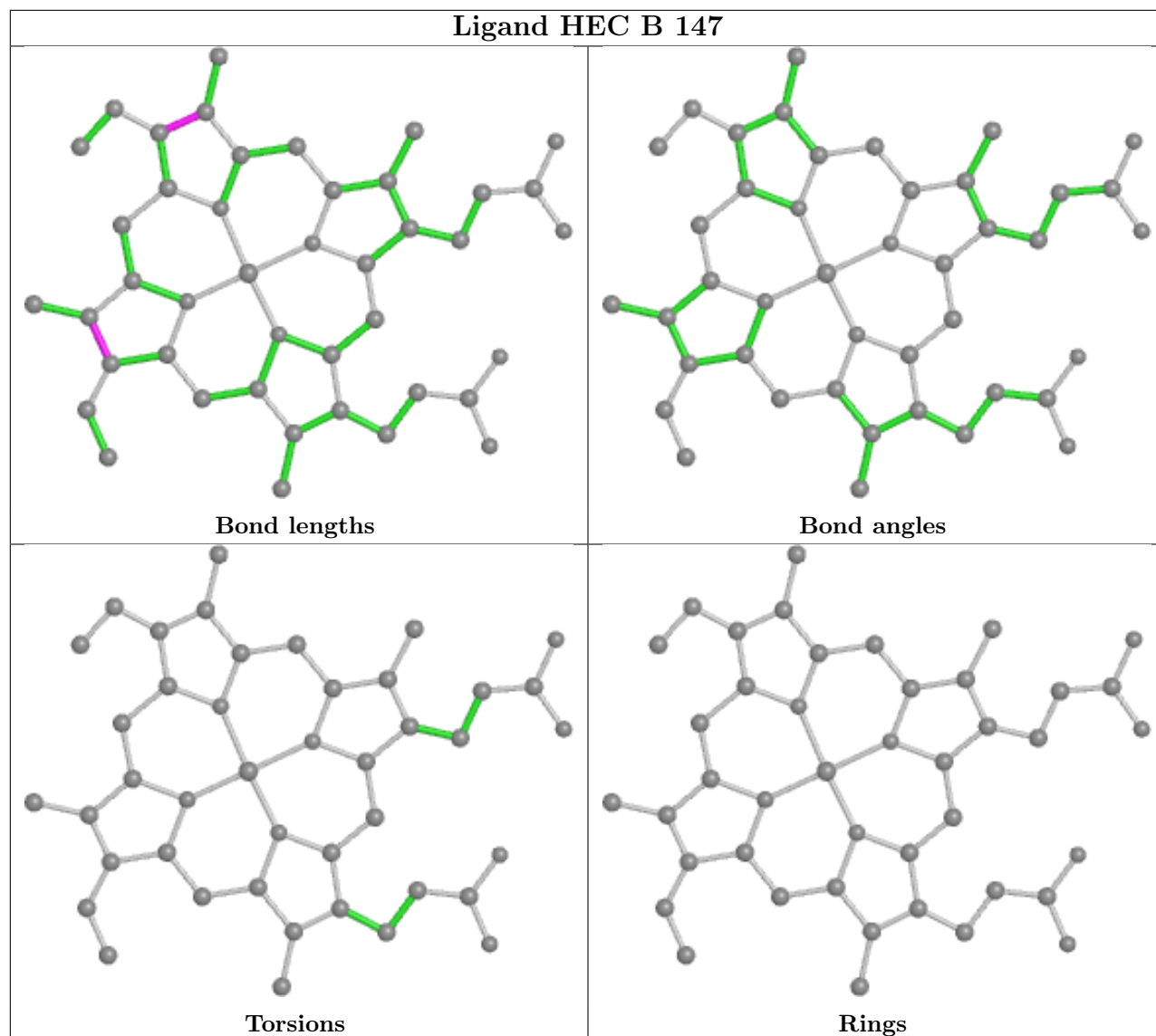
There are no chirality outliers.

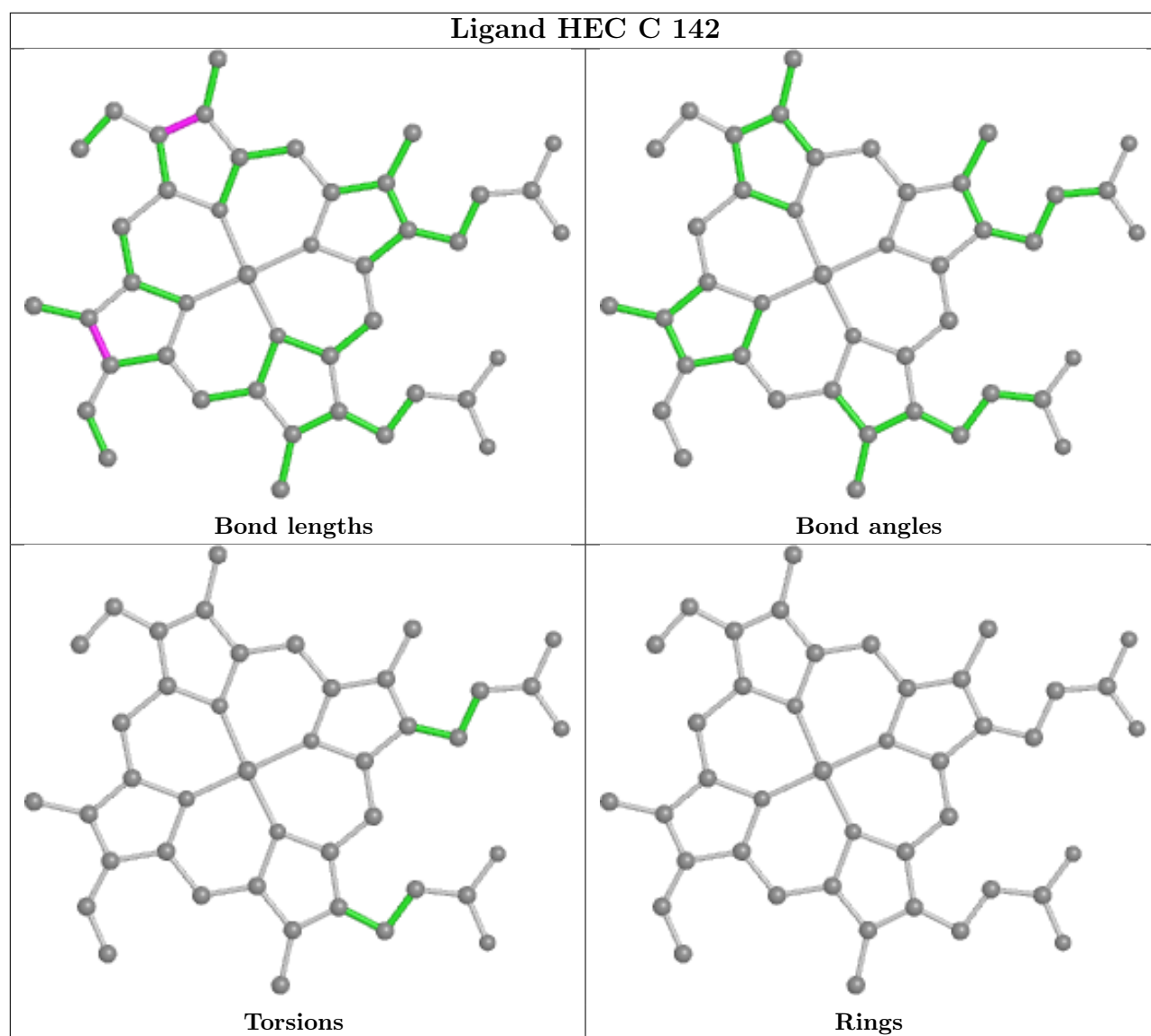
There are no torsion outliers.

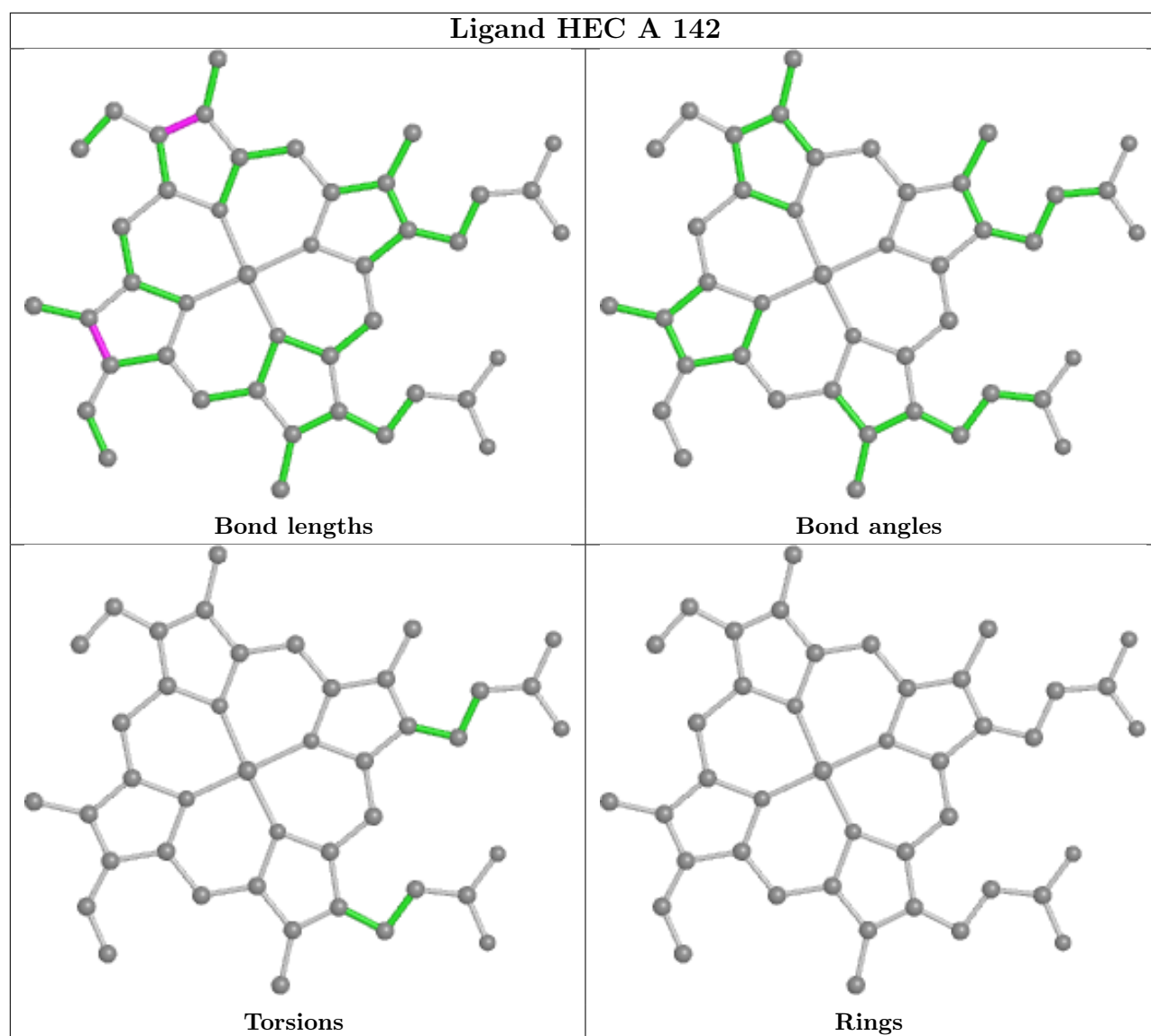
There are no ring outliers.

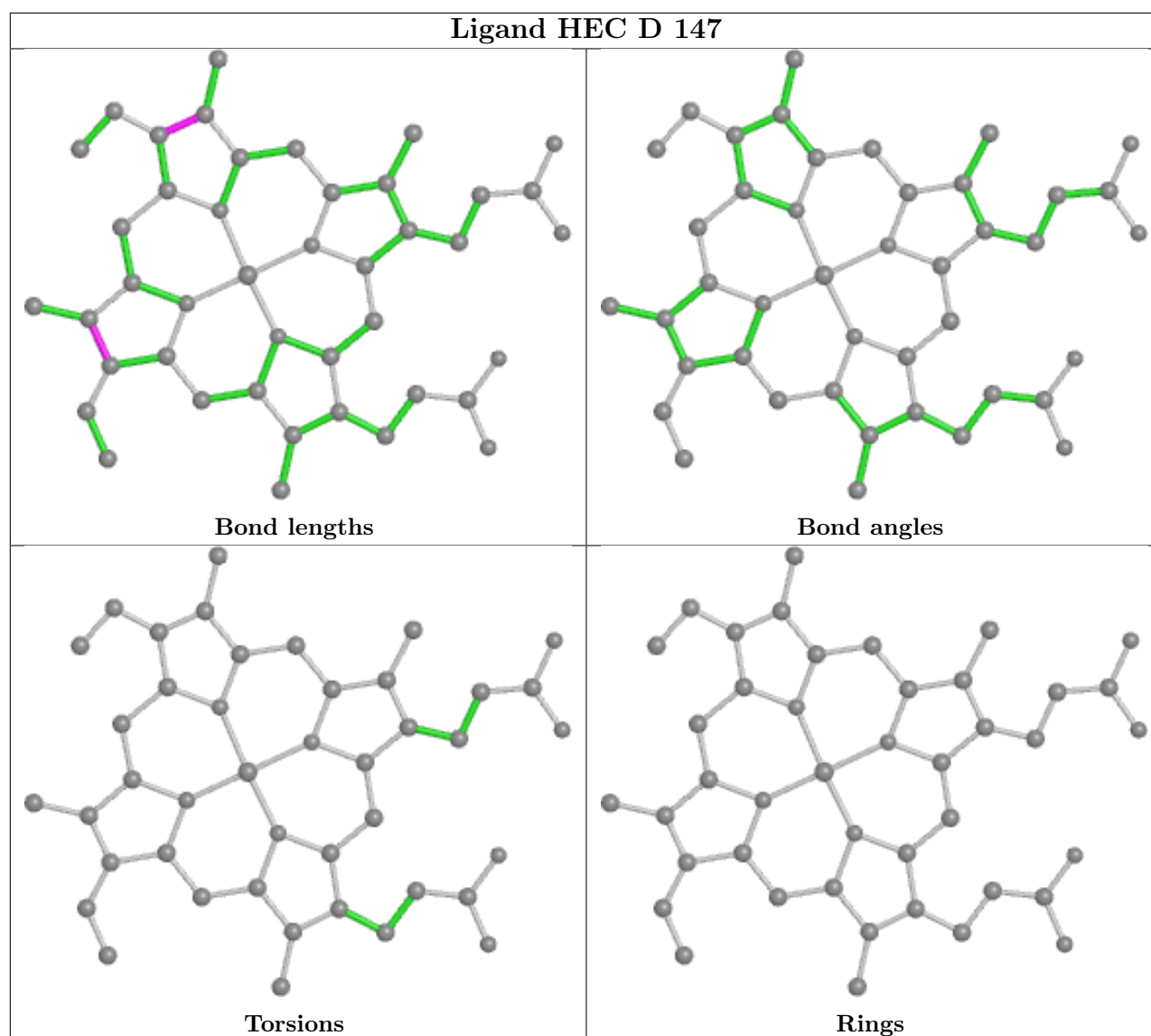
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEC B 147









6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided